Pole structure of the Hamiltonian ζ-function for a singular potential

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Abstract
We study the pole structure of the ζ-function associated with the Hamiltonian H of a quantum mechanical particle living in the half-line $\mathbb{R}^+$, subject to the singular potential $gx^{-2} + x^2$. We show that H admits nontrivial self-adjoint extensions (SAE) in a given range of values of the parameter g. The ζ-functions of these operators present poles which depend on g and, in general, do not coincide with half an integer (they can even be irrational). The corresponding residues depend on the SAE considered.

1. Introduction

In quantum field theory under external conditions, quantities such as effective actions and vacuum energies, which describe the influence of external fields or boundaries on the physical system, are generically divergent and require a renormalization to get a physical meaning.

In this context, a powerful and elegant regularization scheme is based on the use of spectral functions, such as the associated ζ-function [1, 2] and heat-kernel (for recent reviews see, for example, [3–6]).

It is well known [7, 8] that for an elliptic boundary value problem in a ν-dimensional compact manifold with boundary, described by a differential operator A of order ω, with smooth coefficients and defined on a domain of functions subject to local boundary conditions, the ζ-function

$$\zeta_A(s) \equiv \mathrm{Tr}\{A^{-s}\} \tag{1}$$

has a meromorphic extension to the complex s-plane presenting isolated simple poles at $s = (\nu - j)/\omega$, with $j = 0, 1, 2, \ldots$.

In the case of positive definite operators, the ζ-function is related, via Mellin transform, to the trace of the heat-kernel of the problem, $\text{Tr}\{e^{-tA}\}$. The pole structure of $\zeta_A(s)$ determines the small-t asymptotic expansion of this trace [8],

$$\text{Tr}\{e^{-tA}\} \sim \sum_{j=0}^{\infty} a_j(A) t^{(j-\nu)/\omega} \tag{2}$$

where the coefficients are related to the residues by

$$a_j(A) = \text{Res}|_{s=(\nu-j)/\omega} \, \Gamma(s)\zeta_A(s). \tag{3}$$

However, for the case of a differential operator with coefficients presenting singularities, less is known about the structure of the ζ-function or the heat-kernel trace asymptotic expansion.

Callias [9–11] has argued that, when the coefficient in the zeroth-order term in an elliptic, (essentially) self-adjoint, second-order differential operator presents a singularity such as $1/x^2$, the heat-kernel trace asymptotic expansion in terms of powers $t^{(j-\nu)/2}$ (as in (2)) is ill-defined, and an expansion including $\log t$ and perhaps more general powers of t (t^{α} with $\alpha \neq n/2$) would be in order. In particular, considering Hamiltonians H with these characteristics, a small-t asymptotic expansion for the diagonal element $e^{-tH}(x, x)$ has been given in [9, 10] which also presents $t^{(j-\nu)/2} \log t$ terms, and where some of the coefficients are distributions with support concentrated at the singularities.

It is the aim of the present paper to analyse the pole structure of the ζ-function of a Hamiltonian H describing a quantum Schrödinger particle living in the half-line $\mathbb{R}^+$, subject to a singular potential given by $V(x) = gx^{-2} + x^2$, for a real g.[3]

For a certain range of values of g, this Hamiltonian (a second-order differential operator) admits nontrivial self-adjoint extensions[4] in $\mathbf{L}_2(\mathbb{R}^+)$, each one describing a different physical system. We will show that the associated ζ-function presents isolated simple poles which depend on g, which (in general) do not lie at $s = (1 - j)/2$ for $j = 0, 1, \ldots$, and can even be irrational numbers. Moreover, we will find that the residues at these simple poles depend on the self-adjoint extension (SAE) of H considered.

This pole structure for the ζ-function implies a small-t asymptotic expansion for the heat-kernel trace of the problem in terms of powers which (in general) are not half an integer. Moreover, the coefficients in this expansion depend on the selected self-adjoint extension.

The structure of the paper is the following: in section 2 we specify the adjoint of the Hamiltonian operator and in section 3 we determine its deficiency subspaces. The Hamiltonian self-adjoint extensions are characterized in section 4, and in section 5 the corresponding spectrum is described. In section 6 we give an integral representation for the ζ-function of each SAE of the Hamiltonian and in section 7 we discuss the structure of its singularities. In section 8 we analyse some particular cases and establish our conclusions in section 9. Appendix A is devoted to the construction of the closure of H, and in appendix B we outline the necessary asymptotic expansions.

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[3] This potential corresponds to a classically integrable system (see [12], for example). The spectrum of the quantum model subject to Dirichlet boundary conditions has been determined in [13]. This Hamiltonian also appears as an effective radial operator for an isotropic harmonic oscillator in multi-dimensional Euclidean space with given angular momentum eigenvalue [14], a problem for which several results are known: see [14–16] for the heat-kernel and the resolvent in the case of Dirichlet boundary conditions. The resolvent for a different boundary condition could be obtained from this by means of the so-called Krein formula [17, 18]. Our approach to the construction of different SAE of this symmetric Hamiltonian will rather be based on von Neumann's theory [19], after the explicit determination of the deficiency subspaces.

[4] The existence of nontrivial SAE for this kind of singular potential has been pointed out in [20]. SAE with more general singular potentials have also been considered in [21, 22].

2. The Hamiltonian and its adjoint

Let us consider the operator

$$H = -\frac{d^2}{dx^2} + V(x) \tag{4}$$

with

$$V(x) = \frac{g}{x^2} + x^2 \tag{5}$$

densely defined on the domain $\mathcal{D}(H) = \mathcal{C}_0^\infty(\mathbb{R}^+)$, the linear space of functions $\varphi(x)$ with continuous derivatives of all order and compact support not containing the origin. It is easily seen that H is a symmetric operator.

In order to construct the SAE [20] of H we must get its adjoint, $H^\dagger$, and determine the deficiency subspaces.

The operator $H^\dagger$ is defined on the subspace of square-integrable functions $\psi(x)$ for which $(\psi, H\varphi)$ is a continuous linear functional of $\varphi \in \mathcal{D}(H)$. This requires the existence of $\chi(x) \in \mathbf{L}_2(\mathbb{R}^+)$ such that $(\psi, H\varphi) = (\chi, \varphi), \forall \varphi \in \mathcal{D}(H)$. If this is the case, then $\chi(x)$ is uniquely defined, since $\mathcal{D}(H)$ is dense in $\mathbf{L}_2(\mathbb{R}^+)$ and, by definition, $H^\dagger \psi = \chi$.

For $\psi \in \mathcal{D}(H^\dagger)$ and $\forall \varphi \in \mathcal{D}(H)$ we have

$$\begin{aligned}(\psi, H\varphi) &= \int_0^\infty \psi(x)^*(-\varphi''(x) + V(x)\varphi(x)) \, dx \\ &= ((-\psi'' + V(x)\psi), \varphi) = (\chi, \varphi)\end{aligned} \tag{6}$$

where the derivatives of ψ are taken in the sense of distributions.

Equation (6) implies that $\psi''(x) = V(x)\psi(x) - \chi(x)$ is a locally integrable function. Then, its primitive $\psi'(x)$ is absolutely continuous for $x > 0$.

Therefore[5], the domain of $H^\dagger$ is the subspace of square-integrable functions having an absolutely continuous first derivative and such that

$$H^\dagger \psi(x) = -\psi''(x) + V(x)\psi(x) \in \mathbf{L}_2(\mathbb{R}^+) \tag{7}$$

(without requiring any boundary condition at $x = 0$).

In the next section we will determine the deficiency subspaces of H, $\mathcal{K}_\pm = \text{Ker}(H^\dagger \mp i)$.

3. Deficiency subspaces of H

To compute the deficiency indices [19] of H, $n_\pm = \dim \mathcal{K}_\pm$, we must solve the eigenvalue problem

$$H^\dagger \phi_\lambda = -\phi_\lambda''(x) + V(x)\phi_\lambda(x) = \lambda \phi_\lambda \tag{8}$$

for $\phi_\lambda \in \mathcal{D}(H^\dagger)$ and $\lambda \in \mathbb{C}$, with the imaginary part $\text{Im}(\lambda) \neq 0$.

By means of the following ansatz (suggested by the expected behaviour of the solutions of (8) for $x \to 0^+$ and $x \to \infty$),

$$\phi = x^\alpha e^{-\frac{x^2}{2}} F(x^2) \tag{9}$$

with

$$\alpha = 1/2 + \sqrt{g + 1/4} \tag{10}$$

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[5] See proposition 2 on p 150, vol II of [19].

we get from (8) Kummer's equation for $F(z)$:

$$zF''(z) + (b - z)F'(z) - aF(z) = 0 \tag{11}$$

where $a = (2\alpha + 1 - \lambda)/4$ and $b = \alpha + 1/2$.

For real α, we have $g \geqslant -1/4$ and $\alpha \geqslant 1/2$. In this case it can be seen [23] that the only solution of equation (11) leading to a square-integrable at infinity solution of equation (8) is given by the Kummer function $F(z) = U(a; b; z)$. Then, the eigenfunctions of $H^\dagger$ are proportional to

$$\phi_\lambda(x) = x^\alpha \, \mathrm{e}^{-\frac{x^2}{2}} U\left(\frac{2\alpha + 1 - \lambda}{4}; \alpha + \frac{1}{2}; x^2\right). \tag{12}$$

We must now study the behaviour of ϕ_λ near the origin, where $U(a; b; z)$ behaves as $z^{-a}(1 + O(1/z))$ [23]. We must consider two different regions for the parameter α.

For $\alpha \geqslant 3/2, \phi_\lambda \in \mathbf{L}_2(\mathbb{R}^+) \Leftrightarrow a = (2\alpha + 1 - \lambda)/4 = -n$, with $n \in \mathbb{N}$. As a consequence, if $\lambda \notin \mathbb{R}, \phi_\lambda \notin L_2(\mathbb{R}^+)$, and the deficiency subspaces are trivial.

This means that, for $\alpha \geqslant 3/2$, H is essentially self-adjoint, and its discrete spectrum is given by the condition $-a \in \mathbb{N}$, i.e.

$$\lambda_n = 4n + 2\alpha + 1 \tag{13}$$

with $n = 0, 1, 2, \ldots$. The corresponding eigenfunctions are

$$\phi_n = x^\alpha \, \mathrm{e}^{-\frac{x^2}{2}} U\left(-n; \alpha + \tfrac{1}{2}; x^2\right). \tag{14}$$

On the other hand, for $1/2 \leqslant \alpha < 3/2$, one can see [23] that $\phi_\lambda \in L_2(\mathbb{R}^+), \forall \lambda \in \mathbb{C}$. Then, the deficiency subspaces $\mathcal{K}_\pm$ are one-dimensional, and the deficiency indices $n_\pm = 1$.[6] In this region, H admits different self-adjoint extensions.

4. Self-adjoint extensions of H

Since $n_+ = 1 = n_-$ for $1/2 \leqslant \alpha < 3/2$, there exists a one-parameter family of self-adjoint extensions of H, which are in a one-to-one relationship with the isometries from $\mathcal{K}_+$ onto $\mathcal{K}_-$ [19].

The deficiency subspaces $\mathcal{K}_+$ and $\mathcal{K}_-$ are generated by $\phi_+ \equiv \phi_{\lambda=\mathrm{i}}$ and $\phi_- \equiv \phi_{\lambda=-\mathrm{i}} = \phi_+^*$, respectively. Then, each isometry $\mathcal{U}_\gamma : \mathcal{K}_+ \to \mathcal{K}_-$ can be identified with the parameter $\gamma \in [0, \pi)$ defined by

$$\mathcal{U}_\gamma \phi_+ = \mathrm{e}^{-2\mathrm{i}\gamma} \phi_-. \tag{15}$$

The corresponding self-adjoint operator, H_γ, is defined on a dense subspace [19]

$$\mathcal{D}(H_\gamma) \subset \mathcal{D}(H^\dagger) = \mathcal{D}(\overline{H}) \oplus \mathcal{K}_+ \oplus \mathcal{K}_-\tag{16}$$

where $\overline{H}$ is the closure of H. Functions $\phi \in \mathcal{D}(H_\gamma)$ can be written as

$$\phi = \phi_0 + A(\phi_+ + \mathrm{e}^{-2\mathrm{i}\gamma} \phi_-) \tag{17}$$

with $\phi_0 \in \mathcal{D}(\overline{H})$ and A a constant. Since H_γ is a restriction of $H^\dagger$, we have

$$H_\gamma \phi = H^\dagger \phi = \overline{H}\phi_0 + \mathrm{i}A(\phi_+ - \mathrm{e}^{-2\mathrm{i}\gamma} \phi_-). \tag{18}$$

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[6] This is in accordance with Weyl's criterion [19] according to which, for continuous $V(x)$, H is essentially self-adjoint if and only if it is in the limit point case, both at infinity and at the origin. In addition, if $V(x) \geqslant M > 0$, for x large enough, then H is in the limit point case at infinity. In consequence, in the present case H is essentially self-adjoint if and only if it is in the limit point case at zero. In particular, for positive $V(x)$ ($g \geqslant 0$), if $V(x) \geqslant \frac{3}{4}x^{-2}$ for x sufficiently close to zero then H is in the limit point case at the origin. In contrast, if $V(x) \leqslant (\frac{3}{4} - \varepsilon)x^{-2}$, for some $\varepsilon > 0$, then H is in the limit circle case at zero. This confirms our results concerning the self-adjointness of H in different regions of the parameter g.

In the following we take $g \geqslant 0 \Rightarrow 1 \leqslant \alpha < 3/2$. As we will see, condition (17) determines the behaviour of $\phi \in \mathcal{D}(H_\gamma)$ near the origin. Taking the logarithmic derivative of ϕ we get

$$\frac{\phi'}{\phi} = \frac{e^{i\gamma}\phi_0' + 2A\,\mathrm{Re}(e^{i\gamma}\phi_+')}{e^{i\gamma}\phi_0 + 2A\,\mathrm{Re}(e^{i\gamma}\phi_+)}. \tag{19}$$

In this expression, the terms coming from ϕ_+ give the leading contributions for small x. In fact, in appendix A we show that $\phi_0(x) = o(x^\alpha)$ and $\phi_0'(x) = o(x^{\alpha-1})$. Then, for the right-hand side of equation (19) we get [23] (see equation (12))

$$\frac{\phi'(x)}{\phi(x)} = \frac{1-\alpha}{x} + (2\alpha-1)\frac{\Gamma\left(\frac{1}{2}-\alpha\right)}{\Gamma\left(\alpha-\frac{1}{2}\right)}\frac{\cos(\gamma-\gamma_1)}{\cos(\gamma-\gamma_2)}x^{2\alpha-2} + o(x^{2\alpha-2}) \tag{20}$$

where we have $\gamma_1 = \arg\{\Gamma[(-2\alpha+3-i)/4]\}$ and $\gamma_2 = \arg\{\Gamma[(2\alpha+1-i)/4]\}$.

Thus, the limit of equation (19) for $x \to 0^+$ gives the appropriate boundary condition for the functions in the domain of the particular SAE. As we will see, this boundary condition will finally determine a discrete spectrum for H_γ.

5. The spectrum

The boundary condition specified in equation (20) characterizes the domain of a particular SAE of the operator H, H_γ. In order to determine its spectrum, we must find the solutions of (8), ϕ_λ as given in (12) with $\lambda \in \mathbb{R}$, which satisfy this boundary condition. Their behaviour near the origin is given by (see equation (12) and [23])

$$\frac{\phi_\lambda'(x)}{\phi_\lambda(x)} = \frac{1-\alpha}{x} + (2\alpha-1)\frac{\Gamma\left(\frac{1}{2}-\alpha\right)}{\Gamma\left(\alpha-\frac{1}{2}\right)}\frac{\Gamma\left[\frac{2\alpha+1-\lambda}{4}\right]}{\Gamma\left[\frac{-2\alpha+3-\lambda}{4}\right]} \cdot x^{2\alpha-2} + o(x^{2\alpha-2}). \tag{21}$$

Comparison of equations (20) and (21) immediately leads us to

$$\frac{\Gamma\left(\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)} = \beta(\gamma,\kappa) \tag{22}$$

where we have defined the parameters

$$\kappa = \frac{2\alpha+1}{4} = \frac{1}{4}(2+\sqrt{1+4g}) \in [3/4, 1)$$

$$\beta(\gamma,\kappa) = \cos(\gamma-\gamma_1)/\cos(\gamma-\gamma_2). \tag{23}$$

Equation (22) determines a discrete spectrum for each SAE. In figure 1 we plot both sides of equation (22) as a function of λ, for $\kappa = 4/5$ and $\beta = 1$. The abscissae of the intersections of these two functions give the corresponding spectrum.

Note that each SAE can equivalently be characterized by $\beta \in \mathbb{R} \cup \{-\infty\}$. Then, we will also use the notation $H_{(\beta)}$ to design this SAE.

The spectrum of $H_{(\beta)}$ is bounded from below, and presents a negative eigenvalue for those SAE characterized by $\beta > \Gamma(\kappa)/\Gamma(1-\kappa)$ (even though the potential $V(x) \geqslant 2\sqrt{g} \geqslant 0$). Moreover, there is no common lower bound; instead, any negative real is in the spectrum of some SAE.

For any value of g, there are two particular SAE for which the spectrum can be easily worked out (see equation (22)):

- For $\beta = 0$ the spectrum is given by

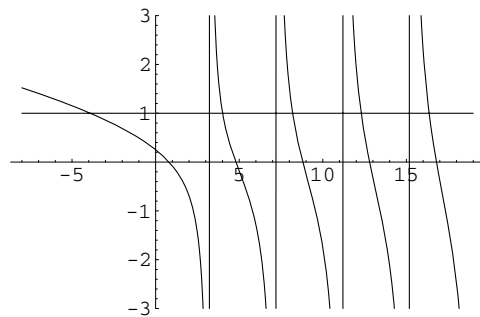$$\lambda_n = 4(n+1-\kappa) \tag{24}$$

  with $n = 0, 1, 2, \ldots$.

Figure 1. $F(\lambda) \equiv \frac{\Gamma(\kappa - \frac{\lambda}{4})}{\Gamma(1 - \kappa - \frac{\lambda}{4})}$ as a function of λ, for $\kappa = 4/5$. The solutions of $F(\lambda) = \beta$ give the spectrum of the SAE identified by β.

- For $\beta = -\infty$ the spectrum is given by

$$\lambda_n = 4(n + \kappa) \tag{25}$$

  with $n = 0, 1, 2, \ldots$.

  For other values of β, the eigenvalues grow linearly with n,

$$4(n - 1 + \kappa) < \lambda_n < 4(n + \kappa). \tag{26}$$

5.1. The case with $g = 0$

It is instructive to consider the particularly simple case of the harmonic oscillator in the half-line, for which there is no singularity in the potential. Indeed, for $g = 0$ ($\alpha = 1$ or $\kappa = 3/4$), the boundary condition (equation (20)) reads

$$\frac{\phi'(x)}{\phi(x)} = -2\beta + O(x) \tag{27}$$

or, equivalently,

$$\lim_{x \to 0^+} \{\phi'(x) + 2\beta\phi(x)\} = 0 \tag{28}$$

which corresponds to Robin boundary conditions at the origin. Dirichlet and Neumann boundary conditions are obtained for $\beta = -\infty$ and $\beta = 0$, respectively.

Let us now study the eigenfunctions and eigenvalues of the self-adjoint extensions of H corresponding to different values of β.

5.1.1. Dirichlet boundary conditions ($\beta = -\infty$). Since $\kappa = 3/4$, the eigenvalues (see equation (25)) are given by

$$\lambda_n = 4n + 3 \tag{29}$$

where $n = 0, 1, 2, \ldots$.

Since the Hamiltonian (equation (4)) corresponds in this case to a particle with mass $m = 1/2$ and frequency $\omega = 2$, the eigenvalues of this SAE can be written as $\lambda_n = \omega[(2n + 1) + 1/2]$, which coincides with the spectrum of the odd parity eigenvectors of the harmonic oscillator on the complete real line.

In fact, the eigenfunctions are given by (see equation (12) and [23])

$$\phi_n = 2^{-2n-1} e^{-\frac{x^2}{2}} H_{2n+1}(x). \tag{30}$$

5.1.2. Neumann boundary conditions ($\beta = 0$). In this case, the eigenvalues (see equation (24)) are given by

$$\lambda_n = 4n + 1 \tag{31}$$

where $n = 0, 1, 2, \ldots$. These eigenvalues can be written as $\lambda_n = \omega(2n+1/2)$, which coincides with the even parity sector of the harmonic oscillator spectrum on the complete real line.

The eigenfunctions are now given by (see equation (12))

$$\phi_n = 2^{-2n} \, \mathrm{e}^{-\frac{x^2}{2}} H_{2n}(x). \tag{32}$$

5.1.3. Robin boundary conditions ($\beta \neq 0, -\infty$). For finite $\beta \neq 0$, the eigenfunctions are given by (equation (12))

$$\phi_\lambda = x \, \mathrm{e}^{-\frac{x^2}{2}} U\left(\frac{3-\lambda}{4}; \frac{3}{2}; x^2\right) \tag{33}$$

and the corresponding eigenvalues are determined by the transcendental equation

$$\frac{\Gamma\left(\frac{3-\lambda}{4}\right)}{\Gamma\left(\frac{1-\lambda}{4}\right)} = \beta(\gamma, 3/4). \tag{34}$$

Note that, for general Robin boundary condition, the ground state is negative (less than the minimum of the potential) for $\beta > \Gamma\left[\frac{3}{4}\right]/\Gamma\left[\frac{1}{4}\right]$.

6. The integral representation for the ζ-function

The spectrum of each SAE of the operator H in (4) is determined by equation (22), for any given $\beta \in [-\infty, \infty)$. In this section, we will study the pole structure of the associated ζ-function, defined as

$$\zeta_\beta(s) \equiv \mathrm{Tr}\left\{H_{(\beta)}^{-s}\right\} = \sum_n \lambda_{\beta,n}^{-s}. \tag{35}$$

Note that, since the eigenvalues grow linearly with n (see equation (26)), $\zeta_\beta(s)$ is analytic in the half-plane $\mathrm{Re}(s) > 1$.

For finite β, let us define the holomorphic function

$$f(\lambda) = \frac{1}{\Gamma\left(1 - \kappa - \frac{\lambda}{4}\right)} - \frac{\beta}{\Gamma\left(\kappa - \frac{\lambda}{4}\right)} \tag{36}$$

with $\frac{3}{4} \leqslant \kappa < 1$. The eigenvalues of the self-adjoint operator $H_{(\beta)}$ correspond to the zeros of $f(\lambda)$ which, consequently, are all real. They are also positive, with the only possible exception of the first one, according to the discussion in the previous section.

Moreover, the zeros of $f(\lambda)$ are simple. To prove this, let us assume that the converse is true, i.e. there is a $\lambda \in \mathbb{R}$ such that $f(\lambda) = f'(\lambda) = 0$. Taking into account

$$\begin{aligned}
f'(\lambda) &= \frac{\psi\left(1 - \kappa - \frac{\lambda}{4}\right)}{4\Gamma\left(1 - \kappa - \frac{\lambda}{4}\right)} - \beta \frac{\psi\left(\kappa - \frac{\lambda}{4}\right)}{4\Gamma\left(\kappa - \frac{\lambda}{4}\right)} \\
&= \frac{1}{4}\left\{\frac{\left[\psi\left(1 - \kappa - \frac{\lambda}{4}\right) - \psi\left(\kappa - \frac{\lambda}{4}\right)\right]}{\Gamma\left(1 - \kappa - \frac{\lambda}{4}\right)} + \psi(\kappa - \lambda/4)\, f(\lambda)\right\}
\end{aligned} \tag{37}$$

where $\psi(z)$ is the polygamma function, we see that our assumption requires

$$\psi(1 - \kappa - \lambda/4) = \psi(\kappa - \lambda/4) \tag{38}$$

which is not the case for any $\lambda \in \mathbb{R}$, if $\frac{3}{4} \leqslant \kappa < 1$.

Therefore, the ζ-function can be represented as the integral on the complex plane,

$$\zeta_\beta(s) = \frac{1}{2\pi i} \oint_C \lambda^{-s} \frac{f'(\lambda)}{f(\lambda)} + \Theta(-\lambda_{0,\beta})\lambda_{0,\beta}^{-s} \tag{39}$$

where C is a curve which encircles the positive zeros of $f(\lambda)$ counterclockwise. In equation (39), $\Theta(y) = 1$ for $y > 0$ and $\Theta(y) = 0$ for $y \leqslant 0$.

Let us consider the dominant asymptotic behaviour of the quotient

$$\frac{f'(\lambda)}{f(\lambda)} = \frac{\left[\psi\left(1 - \kappa - \frac{\lambda}{4}\right) - \psi\left(\kappa - \frac{\lambda}{4}\right)\right]}{4\left(1 - \beta\frac{\Gamma(1 - \kappa - \frac{\lambda}{4})}{\Gamma(\kappa - \frac{\lambda}{4})}\right)} + \frac{1}{4}\psi(\kappa - \lambda/4). \tag{40}$$

For $|\arg(-\lambda)| < \pi$ and $|\lambda| \to \infty$, it is sufficient to write

$$\psi(\kappa - \lambda/4) = \log(-\lambda) + O(1) \tag{41}$$

$$\psi(1 - \kappa - \lambda/4) - \psi(\kappa - \lambda/4) = O(\lambda^{-1}) \tag{42}$$

$$\frac{\Gamma\left(1 - \kappa - \frac{\lambda}{4}\right)}{\Gamma\left(\kappa - \frac{\lambda}{4}\right)} = O(\lambda^{1-2\kappa}). \tag{43}$$

Consequently, for $\text{Re}(s) > 1$ the path of integration in (39) can be deformed to a vertical line, to get

$$\zeta_\beta(s) = \frac{-1}{2\pi i} \int_{-i\infty+0}^{i\infty+0} \lambda^{-s} \frac{f'(\lambda)}{f(\lambda)} \, d\lambda + h(s) \tag{44}$$

where $h(s)$ (the contribution of the negative eigenvalue, if any) is a holomorphic function.

7. Pole structure of the ζ-function

The integral in equation (44) defines $\zeta_\beta(s)$ as an analytic function in the half-plane $\text{Re}(s) > 1$, which can be meromorphically extended to the whole complex s-plane. It can be written as

$$\zeta_\beta(s) = -\frac{1}{2\pi i} \int_i^{i\infty} \frac{f'(\lambda)}{f(\lambda)}\lambda^{-s} \, d\lambda - \frac{1}{2\pi i} \int_{-i\infty}^{-i} \frac{f'(\lambda)}{f(\lambda)}\lambda^{-s} \, d\lambda + h_1(s)$$

$$= -\frac{e^{-is\pi/2}}{2\pi} \int_1^\infty \frac{f'(i\mu)}{f(i\mu)}\mu^{-s} \, d\mu - \frac{e^{is\pi/2}}{2\pi} \int_1^\infty \frac{f'(-i\mu)}{f(-i\mu)}\mu^{-s} \, d\mu + h_1(s) \tag{45}$$

where $h_1(s)$ is a holomorphic function.

In appendix B we work out the asymptotic expansion of $f'(\lambda)/f(\lambda)$, which is given by

$$\frac{f'(\lambda)}{f(\lambda)} \sim \frac{1}{4}\log(-\lambda) + \frac{1}{4}\sum_{k=0}^\infty c_k(\kappa)(-\lambda)^{-k} + \sum_{N=1}^\infty \sum_{n=0}^\infty C_{N,n}(\kappa, \beta)(-\lambda)^{-N(2\kappa-1)-2n-1} \tag{46}$$

where the coefficients $c_k(\kappa)$ are polynomials in κ whose explicit form is not needed for our purposes, and

$$C_{N,n}(\kappa, \beta) = -(4^{2\kappa-1}\beta)^N \left(2\kappa - 1 + \frac{2n}{N}\right) b_n(\kappa, N) \tag{47}$$

with $b_n(\kappa, N)$ defined in equation (B7) (see also equation (B8)).

As can be seen from equation (46), the asymptotic expansion of $f'(\lambda)/f(\lambda)$ contains the logarithmic term $\frac{1}{4}\log(-\lambda)$, and a series of nonpositive integer powers of λ, both coming from the ψ-function in the last term on the right-hand side of (40). There is also a series of decreasing κ-dependent powers of λ, which comes from the first term on the right-hand side of (40).

For the dominant logarithmic term we get from (45)

$$-\frac{1}{8\pi} \int_1^\infty \left[e^{-i\frac{\pi s}{2}} \log\!\left(e^{-i\frac{\pi}{2}}\mu\right) + e^{i\frac{\pi s}{2}} \log\!\left(e^{i\frac{\pi}{2}}\mu\right) \right] \mu^{-s}\, d\mu$$

$$= \frac{\sin\left(\frac{\pi s}{2}\right)}{8\,(s-1)} - \frac{\cos\left(\frac{\pi s}{2}\right)}{4\pi\,(s-1)^2} = \frac{1}{4}\frac{1}{(s-1)} + h_2(s) \tag{48}$$

where $h_2(s)$ is holomorphic. The analytic extension of this term presents a unique simple pole at $s = 1$, with a residue equal to $1/4$.

The remaining terms in the asymptotic expansion of $f'(\lambda)/f(\lambda)$ are of the form $A_j(-\lambda)^{-j}$, for some $j \geqslant 0$ (see equation (46)). Replacing this in equation (45) we get

$$-\frac{A_j}{2\pi} \int_1^\infty \left[e^{-i\frac{\pi}{2}(s-j)} + e^{i\frac{\pi}{2}(s-j)} \right] \mu^{-s-j}\, d\mu = -\frac{A_j}{\pi} \cos\!\left(\frac{\pi}{2}(s-j)\right) \frac{1}{s - (1-j)}$$

$$= -\frac{A_j \sin(\pi j)}{\pi} \frac{1}{s - (1-j)} + h_3(s) \tag{49}$$

where $h_3(s)$ is holomorphic.

So, from each power-dependent term in the asymptotic expansion of $f'(\lambda)/f(\lambda)$, proportional to $(-\lambda)^{-j}$, we get a unique simple pole at $s = 1 - j$, with a residue given by $-(A_j/\pi) \sin(\pi j)$.

Note that this residue vanishes for integer values of j. In particular, this is the case for all the contribution coming from the asymptotic expansion of $\psi(\kappa - \lambda/4)$ in the last term on the right-hand side of equation (40), except for the first one, the logarithmic term leading to equation (48). In fact, this is the only singularity present in the $\beta = -\infty$ and $\beta = 0$ cases (see equation (40)).

But in general, for $\frac{3}{4} \leqslant \kappa < 1$, there are also poles at non-integer values of s, as follows from (46).

In conclusion, besides the pole at $s = 1$ with residue $1/4$, for each pair of integers

$$(N, n) \quad \text{with} \quad N = 1, 2, 3, \ldots \quad \text{and} \quad n = 0, 1, 2, \ldots \tag{50}$$

the ζ-function of the SAE of H characterized by the parameter β, $\zeta_\beta(s)$, has a contribution with a simple pole at the negative value

$$s = -N(2\kappa - 1) - 2n \in \left(-N - 2n, -\frac{N}{2} - 2n \right] \tag{51}$$

with a β-dependent residue given by

$$\text{Res}(\cdot)|_{s=-N(2\kappa-1)-2n} = \frac{(-1)^N}{\pi} C_{N,n}(\kappa, \beta) \sin(2\pi N\kappa). \tag{52}$$

This is our main result, establishing the existence of κ-dependent poles of the ζ-function which, in general, are not located at a half an integer value of s. Moreover, the residues depend on the SAE considered.

Finally, note that when κ is a rational number, there can be several (but a finite number of) pairs (N, n) contributing to the same pole. They must satisfy

$$\frac{n - n'}{N - N'} = \frac{1}{2} - \kappa = -\frac{p}{q} \in (-1/2, -1/4] \tag{53}$$

where $p, q \in \mathbb{N}$.

In contrast, when κ is irrational the poles coming from different pairs (N, n), also irrational, are not coincident.

7.1. Poles and residues of $\zeta_\beta(s)$

Let us recall that the logarithmic term in expansion (46) leads to a pole at $s = 1$ (see equation (48)) with a residue given by

$$\text{Res}(\cdot)|_{s=1} = \tfrac{1}{4} \tag{54}$$

independently of the SAE considered.

The other poles can be organized in sequences characterized by the integer $N = 1, 2, \ldots$. In each sequence, successive poles differ by -2.

For example, the poles corresponding to the pairs $(N = 1, n)$, with $n = 0, 1, 2, \ldots$, are located at (see equation (51))

$$-1 - 2n < s = 1 - 2\kappa - 2n \leqslant -\tfrac{1}{2} - 2n \tag{55}$$

and have residues given by

$$\text{Res}(\cdot)|_{s=1-2\kappa-2n} = -\frac{C_{1,n}(\kappa, \beta)}{\pi} \sin(2\pi\kappa). \tag{56}$$

Similarly, the poles arising from the $(N = 2, n \geqslant 0)$ terms in the asymptotic expansion (46) are located at

$$-2 - 2n < s = 2 - 4\kappa - 2n < -1 - 2n \tag{57}$$

and have residues given by

$$\text{Res}(\cdot)|_{s=2-4\kappa-2n} = \frac{C_{2,n}(\kappa, \beta)}{\pi} \sin(4\pi\kappa). \tag{58}$$

Note that the poles in the Nth sequence have residues proportional to β^N (see equation (47)).

Finally, let us stress that a pole of $\zeta_\beta(s)$ at a non-integer $s = -N(2\kappa - 1) - 2n$, as in (51), implies the presence of a term in the small-t asymptotic expansion of $\text{Tr}\{e^{-tH_{(\beta)}}\}$ of the form

$$A_{[N(2\kappa-1)+2n]} t^{N(2\kappa-1)+2n} \tag{59}$$

with a coefficient related to the residue by

$$A_{[N(2\kappa-1)+2n]} = \Gamma(-N(2\kappa - 1) - 2n) \, \text{Res}\zeta_\beta(s)|_{s=-N(2\kappa-1)-2n}. \tag{60}$$

7.2. ζ-function singularities from the asymptotic expansion of the eigenvalues

The singular behaviour found for $\zeta_\beta(s)$ can be confirmed (at least for the first few poles) by determining from (22) the asymptotic expansion of the eigenvalues $\lambda_{\beta,n}$ for $n \gg 1$. Indeed, one can make the ansatz

$$\frac{\lambda_{\beta,n}}{4} = 1 - \kappa + n + \varepsilon \tag{61}$$

and self-consistently determine ε through successive corrections. For the first terms we get

$$\frac{\lambda_{\beta,n}}{4} \sim 1 - \kappa + n + \frac{\beta}{\pi} \sin(2\pi\kappa) \, n^{1-2\kappa} + \frac{\beta}{\pi}(1 - 3\kappa + 2\kappa^2) \sin(2\pi\kappa) \, n^{-2\kappa}$$
$$- \frac{\beta^2}{2\pi} \sin(4\pi\kappa) \, n^{2-4\kappa} + \cdots \tag{62}$$

where we have retained only powers of n greater than -2. This leads, for the ζ-function in equation (35), to

$$\zeta_\beta(s) \sim 4^{-s}\zeta(s) + s4^{-s}(\kappa - 1)\,\zeta(s + 1) + s(s + 1)\,4^{-s}\frac{(\kappa - 1)^2}{2}\zeta(s + 2)$$

$$- s4^{-s}\frac{\beta}{\pi}\sin(2\kappa\pi)\,\zeta(s + 2\kappa) - s(s + 2\kappa)\,4^{-s}\frac{\beta}{\pi}(\kappa - 1)\sin(2\pi\kappa)\,\zeta(1 + s + 2\kappa)$$

$$+ s4^{-s}\frac{\beta^2}{2\pi}\sin(4\pi\kappa)\,\zeta(s - 1 + 4\kappa) + \cdots \tag{63}$$

where $\zeta(z)$ is the Riemann ζ-function, which presents a unique simple pole at $z = 1$, with a residue equal to 1.

This result shows a pole structure in agreement with the one previously described.

8. Particular cases

In this section we will show how our results reduce to the usual ones for $g = 0$ (when there is no singularity in the potential). We will also show that, for $\beta = 0$ and $\beta = -\infty$, the ζ-function presents a unique simple pole.

8.1. The $\beta = 0$ and $\beta = -\infty$ SAE

The ζ-function for the SAE characterized by $\beta = 0$ and $\beta = -\infty$ can be exactly evaluated, since in these cases the spectrum was explicitly computed in equations (24) and (25) respectively. We get

$$\zeta_0(s) = 4^{-s}\sum_{n=0}^{\infty}(n + 1 - \kappa)^{-s} = 4^{-s}\zeta(s, 1 - \kappa)$$

$$\zeta_{-\infty}(s) = 4^{-s}\sum_{n=0}^{\infty}(n + \kappa)^{-s} = 4^{-s}\zeta(s, \kappa) \tag{64}$$

where $\zeta(s, q)$ is the Hurwitz ζ-function, whose analytic extension presents only a simple pole at $s = 1$, with a residue Res $\zeta(s, q)|_{s=1} = 1$. This leads, in both cases, to a unique simple pole for the ζ-function at $s = 1$, with a residue equal to $1/4$, in agreement with equation (48).

In fact, from equations (52) and (47) it is evident that all the residues corresponding to negative poles vanish for $\beta = 0$. On the other hand, for $\beta = -\infty$, $f'(\lambda)/f(\lambda)$ reduces to $\frac{1}{4}\psi(\kappa - \lambda/4)$ (see equation (40)), and the only term leading to a singularity is the logarithm in the asymptotic expansion (46), as already discussed (see equation (48)).

8.2. The harmonic oscillator in the half-line

For the harmonic oscillator in the half-line ($g = 0$ or $\kappa = 3/4$) we still find a simple pole at $s = 1$, with residue $1/4$ (the only singularity for Dirchlet or Neumann boundary conditions, as previously discussed).

For finite β, the remaining singularities are located at (see equation (51)),

$$s = -\frac{N}{2} - 2n \qquad N = 1, 2, 3, \ldots \quad n = 0, 1, 2, \ldots \tag{65}$$

with residues given by (see equation (52))

$$\text{Res}(\cdot)|_{s=-\frac{N}{2}-2n} = \frac{(-1)^N}{\pi}C_{N,n}(\kappa = 3/4, \beta)\sin\left(\frac{3\pi}{2}N\right) \tag{66}$$

which vanish for even N.

Then, each pole (except for the first one, at $s = 1$) corresponds to a negative half-integer,

$$s = -k - 1/2 \qquad k = 0, 1, 2 \ldots . \tag{67}$$

Moreover, it is clear that for finitely many pairs (N, n) satisfying $N + 4n = 2k + 1$, the corresponding poles lie at the same point.

Therefore, the residue of $\zeta_\beta(s)$ at $s = -k - 1/2$ must be computed by adding all these contributions, characterized by $N = 2(k - 2n) + 1$, with $n = 0, 1, 2, \ldots, [k/2]$. We get

$$\text{Res}(\zeta_\beta(s))|_{s=-k-\frac{1}{2}} = \frac{(-1)^{k+1}}{\pi} \sum_{n=0}^{[k/2]} C_{[2(k-2n)+1],n}(\kappa = 3/4, \beta). \tag{68}$$

For example, for $k = 0$, the residue is

$$\text{Res}(\zeta_\beta(s))|_{s=-\frac{1}{2}} = -\frac{1}{\pi} C_{1,0}(\kappa = 3/4, \beta) = \frac{\beta}{\pi} \tag{69}$$

and, for $k = 1$,

$$\text{Res}(\zeta_\beta(s))|_{s=-\frac{3}{2}} = \frac{1}{\pi} C_{3,0}(\kappa = 3/4, \beta) = -\frac{4}{\pi} \beta^3. \tag{70}$$

9. Conclusions

In this paper we have analysed the pole structure of the ζ-function of the Hamiltonian describing a quantum Schrödinger particle living in the half-line $\mathbb{R}^+$, subject to the singular potential $V(x) = gx^{-2} + x^2$.

We have specified the domain of the adjoint of the Hamiltonian, $H^\dagger$, and determined the deficiency subspaces of H, initially defined on $\mathcal{C}_0^\infty(\mathbb{R}^+)$. We have shown that, for $-1/4 \leqslant g < 3/4$, H admits nontrivial self-adjoint extensions which depend on a continuous real parameter β.

For computational convenience, we have limited our analysis to the range $0 \leqslant g < 3/4$.

Once the closure of H was determined (studied in appendix A), we were able to characterize each SAE $H_{(\beta)}$ by the behaviour (singular, in general) near the origin of the functions in the corresponding domain of definition. This relation also allowed for the identification of the spectrum of $H_{(\beta)}$ with the zeros of an analytic function $f(\lambda)$.

The asymptotic expansion of $f(\lambda)$ (outlined in appendix B) led to the determination of the poles and residues of the ζ-function associated with $H_{(\beta)}$, $\zeta_\beta(s)$.

We have shown that the poles of $\zeta_\beta(s)$ can be organized in sequences characterized by an integer $N = 1, 2, 3, \ldots$, and are located at $s = -N(2\kappa - 1) - 2n$, with $n = 0, 1, 2, \ldots$, and $\kappa = (1 + \sqrt{g + 1/4})/2 \in [3/4, 1)$. Note that these values of s are not, in general, half an integer (which are the expected positions of the poles for a second-order differential operator with smooth coefficients on a compact segment), and they are irrational numbers for irrational values of κ.

We have also found that the residues depend on the parameter β characterizing the SAE $H_{(\beta)}$.

We have confirmed this ζ-function pole structure (for the first poles) through the comparison with the results obtained from the asymptotic behaviour of the eigenvalues.

These results also imply that the small-t asymptotic expansion of the heat-kernel of $H_{(\beta)}$ contains powers of t which (in general) are not half an integer, and that the corresponding coefficients depend on the SAE.

Finally, several particular cases were analysed, finding that our results are consistent with the known ones. In particular, for the harmonic oscillator ($g = 0$) in the half-line, subject to any local boundary condition at $x = 0$, the poles lie at half-integer values of s.

A final remark is in order: note that the unusual pole structure described previously is a consequence of having a potential with a *moderate* singular behaviour near the origin. In fact, for $g \geqslant 3/4$, where the Hamiltonian H is essentially self-adjoint due to a stronger singular behaviour of $V(x)$, the ζ-function simply reduces to $4^{-s}\zeta(s, \kappa)$ (see equation (13)), which presents a unique pole at $s = 1$ with residue $1/4$.

A similar pole structure is obtained for the Hamiltonian ζ-function of charged Dirac particles living in $(2 + 1)$ dimensions, in the presence of both a uniform magnetic field and a singular magnetic tube with a non-integer flux. This problem was considered in [24], where it was shown that the Hamiltonian restricted to a *critical* angular momentum subspace admits nontrivial SAE, whose spectra are determined by a transcendental equation similar to (22). These results will be reported elsewhere.

Acknowledgments

Appendix A. Closure of H

In this section we will justify disregarding the contributions from the functions in the domain of the closure $\overline{H}$ to the boundary condition, equation (20). Indeed, we will show that if $\phi \in \mathcal{D}(\overline{H})$ then

$$\phi(x) = o(x^\alpha) \quad \text{and} \quad \phi'(x) = o(x^{\alpha-1}) \tag{A1}$$

near the origin, for any $\alpha < 3/2$.

In order to determine the closure of Hamiltonian's graph we must consider the Cauchy sequences in $\mathcal{D}(H) = \mathcal{C}_0^\infty(\mathbb{R}^+)$, $\{\varphi_n\}_{n\in\mathbb{N}}$, such that $\{H\varphi_n\}_{n\in\mathbb{N}}$ are also Cauchy sequences. Note that, since the coefficients in H are real (see equation (4)), we can consider real functions.

Let us call $\varphi = \varphi_n - \varphi_m$, with $n, m \in \mathbb{N}$. Then $\varphi \to 0$ and $H\varphi \to 0$ as $n, m \to \infty$.

Consider first the scalar product

$$\begin{aligned}
(\varphi, H\varphi) &= \int_0^\infty \varphi \left(-\varphi'' + \frac{g}{x^2}\varphi + x^2\varphi\right) \mathrm{d}x \\
&= \int_0^\infty \left(\varphi'^2 + \frac{g}{x^2}\varphi^2 + x^2\varphi^2\right) \mathrm{d}x \leqslant \|\varphi\| \, \|H\varphi\| \to 0
\end{aligned} \tag{A2}$$

for $n, m \to \infty$. Therefore, for $g > 0$, we conclude that

$$\{\varphi_n'(x)\}_{n\in\mathbb{N}} \qquad \left\{\frac{\varphi_n(x)}{x}\right\}_{n\in\mathbb{N}} \qquad \text{and} \qquad \{x\varphi_n(x)\}_{n\in\mathbb{N}} \tag{A3}$$

are also Cauchy sequences.

We will now prove the following:

Lemma. *Let $\{\varphi_n\}_{n\in\mathbb{N}}$ be a Cauchy sequence in $\mathcal{D}(H) = \mathcal{C}_0^\infty(\mathbb{R}^+)$ such that, for $g > 0$, $1 \leqslant a < 2$ and $g \neq (a^2 - 1)/4$,*

$$\{H\varphi_n\}_{n\in\mathbb{N}} \qquad \left\{\frac{\varphi_n(x)}{x^a}\right\}_{n\in\mathbb{N}} \qquad \text{and} \qquad \left\{\frac{\varphi_n'(x)}{x^{a-1}}\right\}_{n\in\mathbb{N}} \tag{A4}$$

are also Cauchy sequences. Then,

$$\left\{\frac{\varphi_n(x)}{x^{1+a/2}}\right\}_{n\in\mathbb{N}} \qquad \text{and} \qquad \left\{\frac{\varphi_n'(x)}{x^{a/2}}\right\}_{n\in\mathbb{N}} \tag{A5}$$

are Cauchy sequences too.

Proof. As before, let $\varphi = \varphi_n - \varphi_m$. First note that, for $1 \leqslant a < 2$,

$$\int_0^\infty \left(x^{1-a/2}\varphi(x)\right)^2 dx \leqslant \int_0^1 (\varphi(x))^2 dx + \int_1^\infty (x\varphi(x))^2 dx \leqslant \|\varphi(x)\|^2 + \|x\varphi(x)\|^2. \quad \text{(A6)}$$

Then, from (A3), we see that $\left\{x^{1-a/2}\varphi_n(x)\right\}_{n\in\mathbb{N}}$ is also a Cauchy sequence. A straightforward calculation shows that

$$\left(\frac{\varphi(x)}{x^a}, H\varphi(x)\right) = \int_0^\infty \left\{ \left(\frac{\varphi'(x)}{x^{a/2}}\right)^2 + \left[g - \frac{a(a+1)}{2}\right]\left(\frac{\varphi(x)}{x^{1+a/2}}\right)^2 + \left(x^{1-a/2}\varphi(x)\right)^2 \right\} dx. \quad \text{(A7)}$$

Similarly,

$$\left(\frac{\varphi'(x)}{x^{a-1}}, H\varphi(x)\right) = \int_0^\infty \left\{ -\left(\frac{a-1}{2}\right)\left(\frac{\varphi'(x)}{x^{a/2}}\right)^2 \right.$$

$$\left. + g\left(\frac{a+1}{2}\right)\left(\frac{\varphi(x)}{x^{1+a/2}}\right)^2 + \left(\frac{a-3}{2}\right)\left(x^{1-a/2}\varphi(x)\right)^2 \right\} dx. \quad \text{(A8)}$$

Now, taking into account that the sum of fundamental sequences is also a Cauchy sequence, we see that

$$\left(A\frac{\varphi(x)}{x^a} + B\frac{\varphi'(x)}{x^{a-1}}, H\varphi(x)\right) \to 0 \quad \text{(A9)}$$

when $n, m \to \infty$, for any pair of real numbers A and B.

The coefficients of $\left(\frac{\varphi'(x)}{x^{a/2}}\right)^2$ and $\left(\frac{\varphi(x)}{x^{1+a/2}}\right)^2$ in the expression of the scalar product in (A9) are

$$A - B\left(\frac{a-1}{2}\right) \qquad \text{and} \qquad A\left(g - \frac{a(a+1)}{2}\right) + Bg\left(\frac{a+1}{2}\right) \quad \text{(A10)}$$

respectively. One can see that, by choosing one of them as zero, the other is nonvanishing (except for $g = (a^2 - 1)/4$).

It is easily seen that these results prove the lemma. $\qquad\square$

For $a = 1$, from (A3) and the lemma, we conclude that

$$\left\{\frac{\varphi_n(x)}{x^{3/2}}\right\}_{n\in\mathbb{N}} \qquad \text{and} \qquad \left\{\frac{\varphi_n'(x)}{x^{1/2}}\right\}_{n\in\mathbb{N}} \quad \text{(A11)}$$

are Cauchy sequences.

Let us first suppose that g is an irrational number. Then, applying iteratively the lemma from (A11) one can show that, for any positive integer k,

$$\left\{\frac{\varphi_n(x)}{x^{2[1-(1/2)^k]}}\right\}_{n\in\mathbb{N}} \qquad \text{and} \qquad \left\{\frac{\varphi_n'(x)}{x^{2[1-(1/2)^k]-1}}\right\}_{n\in\mathbb{N}} \quad \text{(A12)}$$

are Cauchy sequences.

Finally, for any given $\varepsilon > 0$ there are integers k_1 and k_2 such that $(1/2)^{k_1} \leqslant \varepsilon \leqslant (1/2)^{k_2}$. Taking into account

$$\begin{aligned} \frac{1}{x^{2-\varepsilon}} &\leqslant \frac{1}{x^{2[1-(1/2)^{k_1}]}} &&\text{for} \quad 0 < x \leqslant 1 \\[2mm] \frac{1}{x^{2-\varepsilon}} &\leqslant \frac{1}{x^{2[1-(1/2)^{k_2}]}} &&\text{for} \quad x \geqslant 1 \end{aligned} \quad \text{(A13)}$$

one immediately concludes that $\left\{\frac{\varphi_n(x)}{x^{2-\varepsilon}}\right\}_{n\in\mathbb{N}}$ is a Cauchy sequence. A similar conclusion is easily obtained for $\left\{\frac{\varphi_n'(x)}{x^{1-\varepsilon}}\right\}_{n\in\mathbb{N}}$.

Let us now suppose that g is a rational number. Then, from (A3) and (A11) it is seen that we can choose an irrational $a \in (1, 3/2)$ from which the lemma can also be applied iteratively to arrive at the same conclusions.

In the following we will consider the behaviour of the functions near the origin.

For any $\varepsilon > 0$, we can write

$$x^{-\alpha}\varphi(x) = \int_0^x (y^{-\alpha}\varphi(y))' \, dy = \int_0^x y^{-\alpha+1-\varepsilon} \left\{ -\alpha \frac{\varphi(y)}{y^{2-\varepsilon}} + \frac{\varphi'(y)}{y^{1-\varepsilon}} \right\} dy. \tag{A14}$$

So, for $x \leqslant 1$, $\alpha < 3/2$ and ε small enough, we have

$$|x^{-\alpha}\varphi(x)| \leqslant \left(\int_0^1 y^{2(-\alpha+1-\varepsilon)} \, dy \right)^{1/2} \left\{ |\alpha| \left\| \frac{\varphi(y)}{y^{2-\varepsilon}} \right\| + \left\| \frac{\varphi'(y)}{y^{1-\varepsilon}} \right\| \right\} \rightarrow_{n,m\to\infty} 0. \tag{A15}$$

Therefore, the sequence $\{x^{-\alpha}\varphi_n(x)\}_{n\in\mathbb{N}}$, with $\alpha < 3/2$, is uniformly convergent in $[0, 1]$, and its limit is a continuous function vanishing at the origin,

$$\lim_{n\to\infty} \left(x^{-\alpha}\varphi_n(x) \right) = x^{-\alpha}\phi(x) \tag{A16}$$

$$\lim_{x\to 0^+} (x^{-\alpha}\phi(x)) = 0. \tag{A17}$$

In particular, for $\alpha = 0$ we have the uniform limit

$$\lim_{n\to\infty} \varphi_n(x) = \phi(x) \tag{A18}$$

which coincides with the limit of this sequence in $\mathbf{L}_2(\mathbb{R}^+)$.

On the other hand, we can also write

$$\int_0^x y^{-\alpha+1} H\varphi(y) \, dy = -x^{-\alpha+1}\varphi'(x) + \int_0^x y^{-\alpha+1-\varepsilon} \left\{ (-\alpha+1)\frac{\varphi'(y)}{y^{1-\varepsilon}} + g\frac{\varphi(y)}{y^{2-\varepsilon}} \right\} dy$$

$$+ \int_0^x y^{-\alpha+2} y\varphi(y) \, dy. \tag{A19}$$

Therefore, for $x \leqslant 1$, $\alpha < 3/2$ and ε sufficiently small, we have

$$|x^{-\alpha+1}\varphi'(x)| \leqslant \left(\int_0^1 y^{2(-\alpha+1)} \, dy \right)^{1/2} \|H\varphi(y)\|$$

$$+ \left(\int_0^1 y^{2(-\alpha+1-\varepsilon)} \, dy \right)^{1/2} \left\{ |\alpha - 1| \left\| \frac{\varphi'(y)}{y^{1-\varepsilon}} \right\| + g \left\| \frac{\varphi(y)}{x^{2-\varepsilon}} \right\| \right\}$$

$$+ \left(\int_0^1 y^{2(-\alpha+2)} \, dy \right)^{1/2} \|y\varphi(y)\| \rightarrow_{n,m\to\infty} 0. \tag{A20}$$

Consequently, the sequence $\left\{ x^{-\alpha+1}\varphi'_n(x) \right\}_{n\in\mathbb{N}}$, with $\alpha < 3/2$, is uniformly convergent in $[0, 1]$, and its limit is a continuous function vanishing at the origin, which we write as $x^{-\alpha+1}\chi(x)$:

$$\lim_{n\to\infty} \left(x^{-\alpha+1}\varphi'_n(x) \right) = x^{-\alpha+1}\chi(x) \tag{A21}$$

$$\lim_{x\to 0^+} (x^{-\alpha+1}\chi(x)) = 0. \tag{A22}$$

In particular, for $\alpha = 1$ we have the uniform limit

$$\lim_{n\to\infty} \varphi'_n(x) = \chi(x) \tag{A23}$$

which coincides with the limit of this sequence in $\mathbf{L}_2(\mathbb{R}^+)$ (see (A3)).

Let us now show that $\chi(x) = \phi'(x)$. Indeed, for $x \leqslant 1$, we have

$$\left| \phi(x) - \int_0^x \chi(y)\,\mathrm{d}y \right| \leqslant |\phi(x) - \varphi_n(x)| + \left| \int_0^x (\chi(y) - \varphi_n'(y))\,\mathrm{d}y \right|$$

$$\leqslant |\phi(x) - \varphi_n(x)| + \|\chi - \varphi_n'\| \to_{n \to \infty} 0. \tag{A24}$$

So, $\phi(x)$ is a differentiable function whose first derivative is $\chi(x)$.

Equations (A17) and (A22) imply that, given $\varepsilon_1 > 0$ and $\alpha < 3/2$,

$$|\phi(x)| < \varepsilon_1 x^\alpha \qquad \text{and} \qquad |\phi'(x)| < \varepsilon_1 x^{\alpha-1} \tag{A25}$$

if $x < \delta$, for some $\delta > 0$ small enough. This proves our assertion.

Appendix B. Asymptotic expansions

In this appendix we will compute the asymptotic expansion for $f'(\lambda)/f(\lambda)$ as given in equation (40).

The asymptotic expansion for the polygamma function appearing on the right-hand side of equation (40) can be easily obtained from Stirling's formula [23],

$$\psi(\kappa - \lambda/4) \sim \log(-\lambda) + \sum_{i=0}^{\infty} c_i(\kappa)(-\lambda)^{-k} \tag{B1}$$

where the coefficients $c_i(\kappa)$ are polynomials in κ which we will not need to explicitly know for our purposes.

On the other hand, taking into account (43), we can write asymptotically for the first term on the right-hand side of equation (40)

$$\frac{\left[\psi\left(1 - \kappa - \frac{\lambda}{4}\right) - \psi\left(\kappa - \frac{\lambda}{4}\right) \right]}{1 - \beta \frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)}} \sim \sum_{N=0}^{\infty} \beta^N \left[\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)} \right]^N \left[\psi\left(1 - \kappa - \frac{\lambda}{4}\right) - \psi\left(\kappa - \frac{\lambda}{4}\right) \right]$$

$$= \sum_{N=0}^{\infty} \beta^N \left[\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)} \right]^N 4 \frac{d}{d(-\lambda)} \log\left[\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)} \right]$$

$$= \sum_{N=0}^{\infty} \frac{\beta^N}{N} 4 \frac{d}{d(-\lambda)} \left[\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)} \right]^N. \tag{B2}$$

From Stirling's formula [23] we get

$$\log\left[\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)} \right] \sim (1 - 2\kappa) \log\left(-\frac{\lambda}{4}\right) + \left\{ \sum_{m=1}^{\infty} a_m(\kappa)(-\lambda)^{-2m} \right\} \tag{B3}$$

where the coefficients in the series are given by

$$a_m(\kappa) = \frac{2^{4m-1}}{2m+1} \left\{ [(1-\kappa)^{2m} - \kappa^{2m}] + \left(\frac{\kappa - 1/2}{m}\right) [(1-\kappa)^{2m} + \kappa^{2m}] \right.$$

$$\left. + (2m+1) \sum_{p=1}^{m} \frac{B_{2p}}{p(2p-1)} \binom{2m-1}{2p-2} \left[\kappa^{2(m-p)+1} - (1-\kappa)^{2(m-p)+1} \right] \right\}. \tag{B4}$$

Then,

$$\left[\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)} \right]^N \sim \left(-\frac{\lambda}{4}\right)^{-N(2\kappa-1)} \sum_{n=0}^{\infty} b_n(\kappa, N)(-\lambda)^{-2n} \tag{B5}$$

where

$$\sum_{n=0}^{\infty} b_n(\kappa, N) z^{-2n} \sim \exp\left(N \sum_{m=1}^{\infty} a_m(\kappa) z^{-2m}\right). \tag{B6}$$

The coefficients $b_n(\kappa, N)$ are polynomials in κ and N given by

$$b_n(\kappa, N) = \sum_{r_1+2r_2+\cdots+nr_n=n} N^{r_1+r_2+\cdots+r_n} \frac{a_1(\kappa)^{r_1} a_2(\kappa)^{r_2} \cdots a_n(\kappa)^{r_n}}{r_1! r_2! \cdots r_n!} \tag{B7}$$

where the sum extends over all sets of non-negative integers $r_1, r_2, \ldots, r_n$ such that $r_1 + 2r_2 + \cdots + nr_n = n$. For the first five coefficients we get

$b_0(\kappa, N) = 1$

$b_1(\kappa, N) = \frac{8}{3} N\kappa(1 - 3\kappa + 2\kappa^2)$

$b_2(\kappa, N) = \frac{32}{45} N\kappa \left(5N\kappa(1 - 3\kappa + 2\kappa^2)^2 + 6(-1 + 10\kappa^2 - 15\kappa^3 + 6\kappa^4)\right)$

$b_3(\kappa, N) = \frac{256}{2835} N\kappa(1 - 3\kappa + 2\kappa^2)(360 - 18(-60 + 7N)\kappa + 35N^2\kappa^2$

$\qquad - 30(72 - 42N + 7N^2)\kappa^3 + 5(216 - 378N + 91N^2)\kappa^4$

$\qquad - 84N(-9 + 5N)\kappa^5 + 140N^2\kappa^6)$ $\tag{B8}$

$b_4(\kappa, N) = \frac{512}{42\,525} N\kappa(1 - 3\kappa + 2\kappa^2)(-45\,360 + 36(-3780 + 221N)\kappa$

$\qquad - 252(60 - 9N + 5N^2)\kappa^2 + 7(32\,400 - 8604N + 540N^2 + 25N^3)\kappa^3$

$\qquad - 315(-240 + 36N - 32N^2 + 5N^3)\kappa^4 + 21(-10\,800 + 9684N$

$\qquad - 2700N^2 + 275N^3)\kappa^5 - 63(-1200 + 3156N - 1420N^2 + 175N^3)\kappa^6$

$\qquad + 6N(9468 - 10\,080N + 1925N^2)\kappa^7 - 1260N^2(-12 + 5N)\kappa^8 + 1400N^3\kappa^9).$

Now, replacing equation (B5) in equation (B2) we get

$$\frac{\left[\psi\left(1 - \kappa - \frac{\lambda}{4}\right) - \psi\left(\kappa - \frac{\lambda}{4}\right)\right]}{4\left[1 - \beta\frac{\Gamma\left(1-\kappa-\frac{\lambda}{4}\right)}{\Gamma\left(\kappa-\frac{\lambda}{4}\right)}\right]}$$

$$\sim -\sum_{N=1}^{\infty} \sum_{n=0}^{\infty} 4^{N(2\kappa-1)} \beta^N \left(2\kappa - 1 + \frac{2n}{N}\right) b_n(\kappa, N)(-\lambda)^{-N(2\kappa-1)-2n-1}$$

$$\equiv \sum_{N=1}^{\infty} \sum_{n=0}^{\infty} C_{N,n}(\kappa, \beta)(-\lambda)^{-N(2\kappa-1)-2n-1}. \tag{B9}$$

Finally, equations (B1) and (B9) lead to the asymptotic expansion of $f'(\lambda)/f(\lambda)$ in equation (46).

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