Weil positivity and Trace formula the archimedean place

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Abstract

We provide a potential conceptual reason for the positivity of the Weil functional using the Hilbert space framework of the semi-local trace formula of [11]. We explore in great details the simplest case of the single archimedean place. The root of this result is the positivity of the trace of the scaling action compressed onto the orthogonal complement of the range of the cutoff projections associated to the cutoff in phase space, for $\Lambda = 1$. We express the difference between the Weil distribution and the trace associated to the above compression of the scaling action, in terms of prolate spheroidal wave functions, and use, as a key device, the theory of hermitian Toeplitz matrices to control that difference. All the concepts and tools used in this paper make sense in the general semi-local case, where Weil positivity implies RH.

Introduction

The Riemann-Weil explicit formula [7] (Appendix B: (149)) is the equality for complex-valued test functions

$$\widehat{f}(\frac{i}{2}) - \sum_{\frac{1}{2}+is\in Z} \widehat{f}(s) + \widehat{f}(-\frac{i}{2}) = \sum_v W_v(f), \quad \widehat{f}(s) := \int_0^\infty f(x)x^{-is}d^*x, \quad d^*x = \frac{dx}{x} \tag{1}$$

where Z is the multi-set of non-trivial zeros of the Riemann zeta function, and v runs over all places $\{\mathbf{R}, 2, 3, 5, \ldots\}$ of $\mathbf{Q}$. For $v = p$, the functional

$$W_p(f) := (\log p) \sum_{m=1}^{\infty} p^{-m/2} \left(f(p^m) + f(p^{-m}) \right) \tag{2}$$

vanishes on test functions with support in (p^{-1}, p), while the archimedean distribution $W_{\mathbf{R}}$ is given by the formula

$$W_{\mathbf{R}}(f) := (\log 4\pi + \gamma)f(1) + \int_1^\infty \left(f(x) + f(x^{-1}) - 2x^{-1/2}f(1) \right) \frac{x^{1/2}}{x - x^{-1}} d^*x. \tag{3}$$

It was shown by A. Weil [35] that the Riemann Hypothesis (RH) is equivalent to the negativity of the right-hand side of (1) as a functional on the convolution algebra of functions on the (locally compact) multiplicative group $\mathbf{R}_+^* = (0, \infty)$. More precisely, following [36], RH is known to be equivalent to the negativity of the right hand side of (1), evaluated on convolutions of

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smooth functions with compact support[1] $g \in C_c^\infty(\mathbf{R}_+^*)$ (with $g^*(x) := \bar{g}(x^{-1})$), and whose Fourier transform vanishes at $\pm\frac{i}{2}$:

$$RH \iff \sum_v W_v(g * g^*) \leqslant 0, \quad \widehat{g}(\pm\frac{i}{2}) = 0. \tag{4}$$

The key point of this equivalence is that the right-hand side of (1), when evaluated on a test function f with compact support, involves only finitely many primes (since W_p vanishes on functions with support in (p^{-1}, p)). Thus, even though the Riemann Hypothesis is concerned with the asymptotic distribution of the primes, the equivalent formulation (4) only involves finitely many primes at a time. In [36] H. Yoshida proved the following result (Theorem 1 in that paper[2])

For any smooth, positive definite function f with support in the interval $(1/2, 2)$ and whose Fourier transform vanishes at $\pm\frac{i}{2}$ one has: $W_\infty(f) \geqslant 0$ where $W_\infty := -W_{\mathbf{R}}$.

The proof is a numerical analysis of the positivity of the Weil functional W_∞ restricted to the interval $(\frac{1}{2}, 2)$, and therefore it does not provide any conceptual reason for this positivity that would have a chance to continue to hold when primes are involved.

The main result of the present paper is the following strengthening of Yoshida's result which also provides an operator theoretic conceptual reason for the positivity of the Weil functional. Let ϑ be the unitary representation of $\mathbf{R}_+^*$ in the Hilbert space $L^2(\mathbf{R})_{\rm ev}$ of square integrable even functions on the real line, given by the scaling:

$$(\vartheta(\lambda)\,\xi)(v) := \lambda^{-1/2}\,\xi(\lambda^{-1}\,v), \qquad \forall \xi \in L^2(\mathbf{R})_{\rm ev}\,. \tag{5}$$

Furthermore, consider the orthogonal projection $\mathbf{S} := \Pi_{S(1,1)}$ of $L^2(\mathbf{R})_{\rm ev}$ on the subspace $S(1,1)$ of functions vanishing identically in the interval $[-1, 1]$ together with their Fourier transform (this subspace is the well-known infinite dimensional Sonin's space whose discovery goes back to the work of N. Y. Sonin in the XIX-th century [31]). Then we have[3]

Theorem 1 *Let $g \in C_c^\infty(\mathbf{R}_+^*)$ have support in the interval $[2^{-1/2}, 2^{1/2}]$ and Fourier transform vanishing at $\frac{i}{2}$ and 0. Then the following inequality holds*

$$W_\infty(g * g^*) \geqslant \mathrm{Tr}(\vartheta(g)\,\mathbf{S}\,\vartheta(g)^*). \tag{6}$$

Notice that even though the scaling action ϑ does not restrict to the Sonin's subspace, it can be "compressed" to this subspace. Indeed, one can associate to a test function $f \in C_c^\infty(\mathbf{R}_+^*)$ the trace $\mathrm{Tr}(\vartheta(f)\,\mathbf{S})$, and one verifies that this functional is positive definite by construction, *without imposing any restriction* on the support of f, since when evaluated on the convolution $f = g * g^* = g^* * g$ it is the trace $\mathrm{Tr}(\vartheta(g)\,\mathbf{S}\,\vartheta(g)^*)$ of a positive operator. This compression of the scaling action is intimately related to the cutoff proposed by M. Berry and J. Keating in [2] of the scaling Hamiltonian. This is discussed in [18] which is also a supporting companion of the present paper. Furthermore, by Theorem 4.6 the positive functional $\mathrm{Tr}(\vartheta(f)\,\mathbf{S})$ differs from W_∞ by an infinitesimal in the sense of the quantized calculus (*i.e.* the operator in $L^2([2^{-1/2}, 2^{1/2}])$ associated to the difference is compact).

For finitely many places, inclusive of the archimedean one, the semi-local trace formula of [11]

[1] For any interval $I \subset \mathbf{R}_+^*$ we let $C_c^\infty(I)$ be the space of smooth functions with compact support on $\mathbf{R}_+^*$ whose support is contained in I

[2] Theorem 1 of *op.cit.* is formulated in terms of periodic test functions, one can show [20] that this nuance does not affect the lower bound of the quadratic form

[3] see Appendix C for some comments on the irrelevance of the additional vanishing at 0

provides a canonical Hilbert space theoretic set-up where the local distributions W_v and their sum appear in their precise form, when computing the trace of the scaling action (of the idele classes) on the semi-local version of the adele class space of $\mathbf{Q}$. It is thus natural to implement the fundamental positivity provided by the Hilbert space and the quantized calculus "machine" in the semi-local framework, applied to a finite set of places $F = \{\infty, 2, 3, \ldots, p\}$, and provide a conceptual reason for the positivity of Weil's functional $W_\infty - \sum_{v=2}^{p} W_v$ evaluated on test functions f fulfilling the condition Support$(f) \subset (p^{-1}, p)$. While the present paper is only concerned with the simplest instance of this strategy, namely the case $p = 2$, we report here that the key property that allows one to combine the semi-local trace formula of [11] with the quantized calculus has been already proven, in the general semi-local case, in the recently published paper [19], together with the existence of the semi-local analogue of (classical) Sonin's spaces.

The present paper was originally motivated by the desire to understand the link between the analytic Hilbert space operator theoretic strategy first proposed in [11], and the geometric approach pursued in the joint work of the two authors [13, 17]. The latter unveiled a novel geometric landscape still in development for an intersection theory of divisors (on the square of the Scaling Site [14]), thus not yet in shape to handle the delicate principal values involved in the Riemann-Weil explicit formula. The first contribution of this paper is to make explicit the relation between the two approaches, thus overcoming the above problem. Indeed, the connection between the operator theoretic and the geometric viewpoints is effected by the Schwartz kernels associated to operators. By implementing the additive structure of the adeles, one sees that the Schwartz kernel of the scaling operator corresponds geometrically to the divisor of the Frobenius correspondence.

Fact *The additive structure of the adeles of* $\mathbf{Q}$ *allows one to write the Schwartz kernel* $k(x,y)$ *of the scaling action* $f(x) \mapsto f(\lambda x)$, $\lambda \in \mathbf{R}_+^*$, *in the form*

$$k(x, y) = \underline{\delta}(\lambda x - y).$$

where $\underline{\delta}$ *denotes the Dirac distribution.*

Indeed, one has

$$\int k(x, y) f(y) dy = \int \underline{\delta}(\lambda x - y) f(y) dy = f(\lambda x).$$

The geometric interpretation of the term

$$\frac{1}{|1 - \lambda|} = \int \underline{\delta}(\lambda x - x) dx = \int k(x, x) dx$$

as the trace of the scaling operator remains formal until one handles the singularity at $\lambda = 1$. This is what we achieve in Section 1. The main idea developed in this section (through the use of Schwartz kernels) is to translate geometrically the quantized calculus (see Appendix D). This means that, rather than viewing its basic constituent, namely the operator H of square 1 (see (158)) as the Hilbert transform, we pass in Fourier and interpret H as a multiplication operator. Then the quantized differential, namely the commutator with H, acquires an explicit geometric meaning. In this way we obtain a direct geometric proof of a key equality in the local trace formula of [11] as revisited in [12], namely the equality

$$W_\infty(f) = -\frac{1}{2} \mathrm{Tr}(\widehat{f} u^* đu) \tag{7}$$

where $u = u_\infty$ is the unitary classically associated to the Fourier transform composed with the inversion ([32] and Appendix E) and $đu$ is the quantized differential of u (Appendix D). The geometric counterpart of the multiplication by $\widehat{f}$ is the convolution operator $\vartheta_{\rm m}(f)$. In Lemma 1.4 *(iii)* we compute the Schwartz kernel of the geometric counterpart $(u^* đu)^g$ of the operator $u^* đu$. It is well known that the trace of an operator with Schwartz kernel $k(x, y)$ is given by the integral of the diagonal values $k(x, x)$ and it corresponds geometrically to the intersection with the diagonal. Moreover, the trace of a product of two operators is given by an integral in the full square. Then, the geometric description of the quantized differential splits the right hand side of (7) as the sum of two contributions corresponding to the two "squares" Δ and Σ in the first quadrant: see Figure 1.

In Section 2 we prove the important fact that the obstruction to obtain Weil's positivity in the local archimedean case is due to the sole contribution of the small square Δ. To isolate this part we introduce the function "trace-remainder"

$$\delta(\rho) := \mathrm{Tr}\left(\left(\vartheta_{\rm m}(\rho^{-1}) - P\vartheta_{\rm m}(\rho^{-1})P\right)\frac{1}{2}\,(u_\infty^* đu_\infty)^g\right) \tag{8}$$

where $\vartheta_{\rm m}$ is the scaling action, and P is the orthogonal projection given as the multiplication operator by the characteristic function of $[1, \infty)$. The compression PTP of an operator T associated to a Schwartz kernel $k(x, y)$ reduces it to the big square Σ. The cyclicity property of the trace then shows that (8) measures the difference between the Schwartz kernel of $(u_\infty^* đu_\infty)^g$ and its compression. We prove, following an idea of [18], the *p*ositivity of the following functional L *w*ithout any restriction on the support of the test functions $f \in C_c^\infty(\mathbf{R}_+^*)$

$$L(f) = D(f) + W_\infty(f), \qquad D(f) := \int f(\rho^{-1})\delta(\rho)d^*\rho. \tag{9}$$

The proof (Proposition 2.2 and Corollary 2.3) is abstract and conceptual and rests on Hilbert space operators.
This result is also checked numerically using the equivalence between positivity in the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$ and pointwise positivity after Fourier transform. Indeed, the Fourier transform of the distribution L in (9) is the function $\hat\delta(t) + 2\theta'(t)$, where $\hat\delta(t) := \int_{\mathbf{R}_+^*} \delta(\rho)\rho^{-it}d^*\rho$ and $\theta'(t)$ is the derivative of the Riemann-Siegel angular function. As shown in Figures 3 and 4 the function $\hat\delta(t) + 2\theta'(t)$ is non-negative. The two graphs displayed in Figures 5 and 6 are very striking: they show that the term $\hat\delta(t)$ compensates almost exactly the part of the graph of $\theta'(t)$ where this function is negative. This derivative is an even function which tends to $+\infty$ as the variable tends to $\pm\infty$. This divergence accounts for the singularity of the distribution W_∞ at $\rho = 1$ and the use of a principal value in its definition. The Fourier transform $\hat\delta(t)$ is also even but tends to 0 as $t \to \pm\infty$. Indeed the function $\delta(\rho)$ can be written explicitly for $\rho \geqslant 1$ as follows

$$\delta(\rho) = 2\rho^{\frac{1}{2}}\left(\frac{\mathrm{Si}(2\pi(1+\rho))}{2\pi(1+\rho)} + \frac{\mathrm{Si}(2\pi(\rho-1))}{2\pi(\rho-1)}\right) \tag{10}$$

where Si is the Sine Integral function (*i.e.* the primitive of $\frac{\sin(x)}{x}$ vanishing at 0). Moreover one also has $\delta(\rho^{-1}) = \delta(\rho)$. Its graph (see Figure 2) displays the jump in the derivative $\delta'(\rho)$ from the value -1 as $\rho \to 1^-$ to the value 1 as $\rho \to 1^+$. In Section 3 we explain in details why the behavior of $\delta(\rho)$ at $\rho = 1$ plays a decisive role. Indeed, we prove that by imposing on the test functions the vanishing conditions

$$\widehat{f}(\pm\frac{i}{2}) = \int f(\rho)\rho^{\pm\frac{1}{2}}d^*\rho = 0 \tag{11}$$

amounts, *w*ithout changing the support condition for test functions, to replace $\delta(\rho)$ by $Q\delta(\rho)$, where[4] $Q = -(\rho\partial_\rho)^2 + \frac{1}{4}$. Thus the jump in the derivative $\delta'(\rho)$ at $\rho = 1$ generates $-2\underline{\delta}_1$ where $\underline{\delta}_1$ is the Dirac distribution at $\rho = 1$. This fact, together with the smoothness of $\delta(\rho)$ outside 1 suffices to show, on abstract grounds, that the functional $D \circ Q(f) := \int f(\rho^{-1})Q\delta(\rho)d^*\rho$ is essentially negative (in the sense of convolution) on the subspace $C_c^\infty(I) \subset C_c^\infty(\mathbf{R}_+^*)$ of functions with support contained in a fixed compact interval I. More precisely the operator in the Hilbert space $L^2(\sqrt{I}, d^*\rho)$ associated to $D \circ Q(g * g^*)$ (for g with support in $\sqrt{I}$) admits the decomposition $-2\,\mathrm{Id} + K$ where K is a compact operator of Hilbert-Schmidt class (Theorem 3.6). Hence, by imposing finitely many linear conditions (*i.e.* by restricting to a subspace of $L^2(\sqrt{I}, d^*\rho)$ of finite codimension), one obtains a negative quadratic form. Thus, by applying the same conditions one obtains the positivity of the Weil distribution $W_\infty = L - D$.

In Section 4 we perform a main construction whose effect is that to "move" the small square Δ inside Σ, in order to use the (infinite) reservoir of positivity attached to Σ and thus reducing the contribution of D. For this part we apply the technique of pairs of projections and of prolate functions as introduced in [11]. The key elements are the orthogonal projections $\mathcal{P}_\Lambda$ and $\widehat{\mathcal{P}}_\Lambda$, associated to the cutoff parameter Λ ([12] Chapter 2, §3.3) for $\Lambda = 1$. In Lemma 4.1 we show that for $\rho \geqslant 1$ one has

$$\delta(\rho) = \mathrm{Tr}\left(\vartheta_{\mathrm{m}}(\rho^{-1})\widehat{\mathcal{P}}_1\,\mathcal{P}_1\right) \tag{12}$$

where the right hand side is expressed as a sum of coefficients[5] of the scaling action on prolate spheroidal functions[6]. The process of "moving" Δ inside Σ is performed by implementing the decomposition into irreducible components of the unitary representation of the infinite dihedral group $\mathbf{Z} \ltimes \mathbf{Z}/2\mathbf{Z}$ associated to the pair of projections $\widehat{\mathcal{P}}_1$, $\mathcal{P}_1$. In the non-trivial part given by the range of $\mathcal{P}_1 \vee \widehat{\mathcal{P}}_1$, these irreducible components are two dimensional and labeled by the eigenvalues of the prolate differential operator (see [11] and [12]). The orthogonal space to the range of $\mathcal{P}_1 \vee \widehat{\mathcal{P}}_1$ is the infinite dimensional Sonin's space $S(1,1)$ where the representation is trivial. As we wrote above, the outcome of moving Δ inside Σ has the advantage of reducing the contribution of D using the positivity of $\mathrm{Tr}(\vartheta(h)\mathbf{S})$, where $\mathbf{S} = \Pi_{S(1,1)}$ is the projection onto $S(1,1)$. The main outcome is the following (Theorem 4.6)

Theorem 2 *The functional* $\mathrm{Tr}(\vartheta(f)\mathbf{S})$ *is positive and one has*

$$\mathrm{Tr}(\vartheta(f)\mathbf{S}) = W_\infty(f) + \int f(\rho)\epsilon(\rho)d^*\rho, \qquad \forall f \in C_c^\infty(\mathbf{R}_+^*), \tag{13}$$

where $\epsilon(\rho^{-1}) = \epsilon(\rho)$, $\rho \in \mathbf{R}_+^*$, *and with* $\epsilon(\rho)$ *given, for* $\rho \geqslant 1$, *by*

$$\epsilon(\rho) = \sum \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}\langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle. \tag{14}$$

We refer to Section 4 for the notations and the precise definition of the vectors ζ_n, ξ_n in terms of prolate functions. They correspond respectively to the radial and angular prolate functions.

In Section 5 we analyze the functional $E \circ Q(h) = \int h(\rho^{-1})Q\epsilon(\rho)d^*\rho$. The function $\epsilon(\rho)$ behaves, at $\rho = 1$, similarly to the function $\delta(\rho)$. One has $\epsilon(\rho^{-1}) = \epsilon(\rho)$ and the value of the derivative $\epsilon'(1^+)$ is approximately 22.9965. It follows, likewise for $\delta(\rho)$, that the operator, in the

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[4] The role of the operator Q is to multiply the Fourier transforms of the test functions by $z^2 + \frac{1}{4}$ so that they then vanish at $z = \pm\frac{i}{2}$, thus imposing the boundary conditions while keeping positivity and support restrictions

[5] in the sense of representation theory

[6] The equality (12) provides in particular the link between the geometric square Δ and the single "quantum cell" that was protruding in Figure 5 of [18] in relation to the absorption-emission discussion

Hilbert space $L^2(\sqrt{I}, d^*\rho)$, associated to the functional $E \circ Q$, decomposes as $-2\epsilon'(1^+)\,(\mathrm{Id} - K)$, where K is a compact operator associated to a Hilbert-Schmidt kernel. The functional $E \circ Q$ is thus essentially negative on the space of functions with support contained in a fixed compact interval I.

Section 6 is the final technical part of this paper and is entirely dedicated to the computation of the spectrum of the compact operator K when $I = [\frac{1}{2}, 2]$. The strategy developed in this part is summarized by the following steps

1. Discretize the group $\mathbf{R}_+^*$ by approximating it with $q^{\mathbf{Z}}$, where $q \to 1^+$.
2. Identify the approximating operator K_q used in 1. as a Toeplitz matrix and compute numerically its eigenvalues.
3. Apply the general theory of Toeplitz matrices to rewrite K_q in canonical form.
4. Guess a formula for the operator K independently of q, by comparing its approximate behavior for different values of $q \to 1^+$.
5. Construct a finite rank operator T that provides a good approximation of K on $L^2(\sqrt{I}, d^*\rho)$ for $I = [\frac{1}{2}, 2]$.
6. Compute the spectrum of T and identify the single eigenvector which, after conditioning, makes the functional $E \circ Q$ negative.

The first step is in line with the results of [14, 15] providing a Hasse-Weil formula, in the limit of $\mathbf{F}_q$ as $q \to 1^+$, for the complete Riemann zeta function. The key observation in 2. is that, for $q \sim 1$, the operator K_q has only one eigenvalue > 1. The method used in 2. and 3. is closely related to the technique applied in [23] in the context of RH for curves over finite fields. Step 4. provides an explicit approximation of the function $Q\epsilon(\rho)$ on the relevant interval $I = [\frac{1}{2}, 2]$ which in turns gives, in 5., an approximation of K on $L^2(\sqrt{I}, d^*\rho)$ by a finite rank operator. Step 6. keeps track of the eigenvector associated to the only eigenvalue of K which is > 1. Finally, this process allows one, by conditioning on the orthogonality to this vector (or a sufficiently nearby one), to lower the value of the maximal eigenvalue of K to < 1, thus getting the positivity of $\mathrm{Id} - K$ that in turns yields Theorem 1 and its refinement Theorem 6.11.

1. Geometric interpretation of $\mathrm{Tr}(\widehat{f}\, u^* đu)$

In this section we give a geometric proof of the local trace formula at the archimedean place [11, 12], namely the equality for the local term ($W_{\mathbf{R}} = -W_\infty$)

$$W_{\mathbf{R}}(f) = \frac{1}{2}\mathrm{Tr}(\widehat{f}\, u^* đu) \tag{15}$$

where $\widehat{f}$ is the Fourier transform of a test function $f \in C_c^\infty(\mathbf{R}_+^*)$, $u = u_\infty$ is the unitary classically associated with the Fourier transform composed with the inversion (see [32] and Appendix E) and $đu$ is the quantized differential of u.

The main effect of this geometric proof is to decompose the right hand side of (15) in two terms corresponding to the contributions of the two squares Δ and Σ of Figure 1. We normalize the inner product in $L^2(\mathbf{R})_{\mathrm{ev}}$ as follows

$$\langle \eta \mid \xi \rangle := \frac{1}{2}\int_{\mathbf{R}} \overline{\eta(x)}\xi(x)dx = \int_0^\infty \overline{\eta(x)}\xi(x)dx. \tag{16}$$

We first relate the trace computations performed in $L^2(\mathbf{R})_{\mathrm{ev}}$ with those done in the isomorphic

Hilbert space $L^2(\mathbf{R}_+^*, d^*\lambda)$ using the unitary isomorphism

$$w : L^2(\mathbf{R})_{\rm ev} \to L^2(\mathbf{R}_+^*, d^*\lambda), \qquad (w\xi)(\lambda) := \lambda^{\frac{1}{2}}\xi(\lambda). \tag{17}$$

Given an operator T in $L^2(\mathbf{R})_{\rm ev}$, we shall denote the corresponding operator in $L^2(\mathbf{R}_+^*)$ by

$$T^w := wTw^{-1}. \tag{18}$$

The following lemma provides the description (of the multiplicative version) of the Schwartz kernel of an operator in $L^2(\mathbf{R})_{\rm ev}$ after implementing the isomorphism w

Lemma 1.1 *Let T be an operator in $L^2(\mathbf{R})_{\rm ev}$ of the form*

$$T\xi(x) = \int_{y\geqslant 0} k(x,y)\xi(y)dy, \qquad \forall x \geqslant 0, \quad \forall \xi \in L^2(\mathbf{R})_{\rm ev}. \tag{19}$$

Then the Schwartz kernel of $T^w = wTw^{-1}$ in $L^2(\mathbf{R}_+^*)$ takes the following form

$$k^w(\lambda,\mu) = \lambda^{\frac{1}{2}}\mu^{\frac{1}{2}}k(\lambda,\mu). \tag{20}$$

Moreover, the trace of T, namely $\int_{x\geqslant 0} k(x,x)dx$, is equal to $\int k^w(\lambda,\lambda)d^*\lambda$.

Proof. Since the two Hilbert spaces are isomorphic, one can start with the expression of wTw^{-1} in $L^2(\mathbf{R}_+^*)$ as

$$wTw^{-1}(\eta)(\lambda) := \int_{\mathbf{R}_+^*} k^w(\lambda,\mu)\eta(\mu)d^*\mu.$$

Then, with $\eta = w\xi$ one has $\eta(\mu)d^*\mu = \xi(\mu)\mu^{-1/2}d\mu$, for $x = \lambda > 0$ and $y = \mu$ one gets

$$T\xi(x) = x^{-1/2}\int_{y>0} k^w(x,y)y^{-1/2}\xi(y)dy, \qquad \forall x > 0, \ \xi \in L^2(\mathbf{R})_{\rm ev}.$$

This shows that $k(x,y) = x^{-1/2}k^w(x,y)y^{-1/2}$ and (20) holds. □

Remark 1.2 *In general, an operator T in $L^2(\mathbf{R})$ restricts to $L^2(\mathbf{R})_{\rm ev}$ if it commutes with the symmetry $s\xi(x) = \xi(-x)$. For T with Schwartz kernel $t(x,y)$, i.e. $T\xi(x) = \int_{\mathbf{R}} t(x,y)\xi(y)dy$, this means that $t(-x,-y) = t(x,y)$. The restriction $T_{\rm ev}$ of T to $L^2(\mathbf{R})_{\rm ev}$ is of the form (19) with $k(x,y) = t(x,y) + t(x,-y)$. Its trace is*

$$\mathrm{Tr}(T_{\rm ev}) = \int_{x\geqslant 0} k(x,x)dx = \int_{x\geqslant 0}(t(x,x)+t(x,-x))dx = \frac{1}{2}\int_{\mathbf{R}}(t(x,x)+t(x,-x))dx$$

which is the trace of the composition of T with the projection $\frac{1}{2}(1+s)$.

We define the duality $\langle \mathbf{R}_+^*, \mathbf{R}\rangle$ by the bi-character of $\mathbf{R}_+^* \times \mathbf{R}$

$$\mu(v,s) = v^{-is}, \quad \forall v \in \mathbf{R}_+^*, s \in \mathbf{R}. \tag{21}$$

In the following part we make systematic use of the Fourier transform

$$\mathbf{F}_\mu : L^2(\mathbf{R}_+^*) \to L^2(\mathbf{R}), \qquad \mathbf{F}_\mu(f)(s) := \int_0^\infty f(v)v^{-is}d^*v\,. \tag{22}$$

Given an operator T in $L^2(\mathbf{R})$, we denote the corresponding[7] operator in $L^2(\mathbf{R}_+^*)$ by

$$T^g := \mathbf{F}_\mu^{-1} \circ T \circ \mathbf{F}_\mu. \tag{23}$$

[7] the upper index g stands for "geometric"

Next, we use the quantized calculus technique as in [12] (Chapter 2, §5.1).

We first recall Lemma 2.20 of *op.cit.* which uses the unitary inversion operator I that performs the change of variable $\lambda \to \lambda^{-1}$, in $L^2(\mathbf{R}_+^*)$. We let $\mathbf{F}_{e_\mathbf{R}}$ denote the Fourier transform with respect to the basic character $e_\mathbf{R}(x) = e^{-2\pi i x}$: it defines the unitary in $L^2(\mathbf{R})_{\rm ev}$

$$\mathbf{F}_{e_\mathbf{R}}(\xi)(y) := \int_{-\infty}^{\infty} \xi(x)\, e^{-2\pi i x y}\, dy. \tag{24}$$

On implementing the isomorphism w we obtain

Lemma 1.3 *One has: $\mathbf{F}_{e_\mathbf{R}}^w = I \circ u_\infty^g$. Equivalently, the following equality holds in $L^2(\mathbf{R})_{\rm ev}$*

$$\mathbf{F}_{e_\mathbf{R}} = w^{-1} \circ I \circ \mathbf{F}_\mu^{-1} \circ u_\infty \circ \mathbf{F}_\mu \circ w, \tag{25}$$

where u_∞ is the multiplication operator by the function

$$u_\infty(s) := e^{2\, i\, \theta(s)}, \tag{26}$$

and $\theta(s)$ is the Riemann-Siegel angular function recalled in equation (155) *of Appendix B.*

From the proof of the lemma given in *op.cit.* , we extract and include the following part since it plays a key role in this paper. The Fourier transform $\mathbf{F}_{e_\mathbf{R}}$ preserves globally $L^2(\mathbf{R})_{\rm ev}$. For $\xi \in L^2(\mathbf{R}_+^*)$, one has

$$\begin{aligned}(w \circ \mathbf{F}_{e_\mathbf{R}} \circ w^{-1})(\xi)(v) &= v^{1/2} \int_\mathbf{R} |x|^{-1/2}\, \xi(|x|)\, e^{-2\pi i x v}\, dx \\ &= v^{1/2} \int_{\mathbf{R}_+^*} u^{1/2}\, \xi(u)\, (e^{2\pi i u v} + e^{-2\pi i u v})\, d^*u\,.\end{aligned}$$

Using the inversion I in $L^2(\mathbf{R}_+^*)$, this gives

$$\begin{aligned}(I \circ w \circ \mathbf{F}_{e_\mathbf{R}} \circ w^{-1})(\xi)(\lambda) &= (w \circ \mathbf{F}_{e_\mathbf{R}} \circ w^{-1})(\xi)(\lambda^{-1}) \\ &= \lambda^{-1/2} \int_{\mathbf{R}_+^*} (e^{2i\pi\mu\lambda^{-1}} + e^{-2i\pi\mu\lambda^{-1}})\, \mu^{1/2}\xi(\mu) d^*\mu.\end{aligned}$$

The following lemma provides the description of the Schwartz kernels in $L^2(\mathbf{R}_+^*)$ of several relevant operators

Lemma 1.4 *(i) The Schwartz kernel in $L^2(\mathbf{R}_+^*)$ of the convolution operator u_∞^g is given by*

$$k^u(\lambda, \mu) = 2\lambda^{-\frac{1}{2}}\mu^{\frac{1}{2}} \cos(2\pi\mu/\lambda) \tag{27}$$

(ii) The Schwartz kernel in $L^2(\mathbf{R}_+^*)$ of the operator $(\frac{1}{2}đu_\infty)^g = [P, u_\infty^g]$ is

$$(P(\lambda) - P(\mu))k^u(\lambda, \mu), \quad \text{with} \quad P(v) = \begin{cases} 1 & \text{if } v \geqslant 1, \\ 0 & \text{if } v < 1. \end{cases} \tag{28}$$

(iii) The Schwartz kernel in $L^2(\mathbf{R}_+^*)$ of the operator $(\frac{1}{2}\, u_\infty^* đu_\infty)^g$ is

$$\ell(\nu, \mu) = \int k^u(\lambda, \nu)(P(\lambda) - P(\mu))k^u(\lambda, \mu) d^*\lambda. \tag{29}$$

Proof. (i) Equality (27) follows from the fact that the convolution operator $\mathbf{F}_\mu^{-1} \circ u_\infty \circ \mathbf{F}_\mu$ associated to u_∞ can be written as $I \circ w \circ \mathbf{F}_{e_\mathbf{R}} \circ w^{-1}$, by implementing (25).
(ii) follows from the equality $H^g = 2P - 1$, where H is the operator defining the quantized

differential *i.e.* the Hilbert transform. Moreover, recall that for T with Schwartz kernel k, the kernel of the commutator $[P,T]$ is $(P(\lambda)-P(\mu))k(\lambda,\mu)$.
(iii) One derives (29) by recalling that the Schwartz kernel of the adjoint of an operator with kernel $k(\lambda,\mu)$ is $\overline{k(\mu,\lambda)}$, and that the kernel of the composite T_1T_2 is $\int k_1(\nu,\lambda)k_2(\lambda,\mu)d^*\lambda$. □

Next, we change variables in (29) by letting $y=1/\lambda$. The geometric meaning of this operation is reflected in the appearance of the two squares Δ and Σ as in Figure 1. We obtain

$$\begin{aligned}\ell(\nu,\mu) &= \int k^u(\lambda,\nu)(P(\lambda)-P(\mu))k^u(\lambda,\mu)d^*\lambda = \\ &= 4\mu^{\frac12}\nu^{\frac12}\int \lambda^{-\frac12}\cos(2\pi\nu/\lambda)\lambda^{-\frac12}\cos(2\pi\mu/\lambda)(P(\lambda)-P(\mu))d^*\lambda = \\ &= 4\mu^{\frac12}\nu^{\frac12}\int \cos(2\pi\nu y)\cos(2\pi\mu y)(P(1/y)-P(\mu))dy.\end{aligned}$$

Let $\vartheta_{\rm m}$ be the regular representation of $\mathbf{R}_+^*$ on $L^2(\mathbf{R}_+^*)$

$$(\vartheta_{\rm m}(\lambda)\,\xi)(v) := \xi(\lambda^{-1}\,v), \qquad \forall \xi\in L^2(\mathbf{R}_+^*)\,. \tag{30}$$

The following result provides the description of the distribution $W_{\mathbf{R}}$ as stated at the beginning of this section

Proposition 1.5 *(i) The Schwartz kernel in $L^2(\mathbf{R}_+^*)$ of the operator $\vartheta_{\rm m}(\rho^{-1})(\frac12\, u_\infty^* đu_\infty)^g$ is*

$$\ell_\rho(\nu,\mu) = 4\rho^{\frac12}\mu^{\frac12}\nu^{\frac12}\int \cos(2\pi\rho\nu y)\cos(2\pi\mu y)(P(1/y)-P(\mu))dy \tag{31}$$

(ii) The trace of the operator $\vartheta_{\rm m}(\rho^{-1})(\frac12\, u_\infty^* đu_\infty)^g$ is formally given by

$$\tau(\rho) = 4\rho^{\frac12}\int_{\substack{x>0\\ y>0}} \cos(2\pi\rho x y)\cos(2\pi x y)(P(1/y)-P(x))dydx \tag{32}$$

(iii) The equality (32) defines a distribution τ such that

$$W_{\mathbf{R}}(f) = \int f(\rho^{-1})\tau(\rho)d^*\rho. \tag{33}$$

(iv) For $f\in C_c^\infty(\mathbf{R}_+^*)$ the operator $\vartheta_{\rm m}(f)\frac12(u_\infty^* đu_\infty)^g$ is of trace class and its trace is given by

$$\operatorname{Tr}\left(\vartheta_{\rm m}(f)\frac12(u_\infty^* đu_\infty)^g\right) = \int f(\rho^{-1})\tau(\rho)d^*\rho. \tag{34}$$

Proof. (i) follows from the equality $\ell_\rho(\nu,\mu)=\ell(\rho\nu,\mu)$. More generally, for T with Schwartz kernel k in $L^2(\mathbf{R}_+^*)$, the Schwartz kernel of $(\vartheta_{\rm m}(\rho^{-1})\circ T)$ in $L^2(\mathbf{R}_+^*)$ is $k(\rho a,b)$ since

$$((\vartheta_{\rm m}(\rho^{-1})\circ T)\xi)(a) = (T\xi)(\rho a) = \int k(\rho a,b)\xi(b)d^*b.$$

(ii) follows from (i), using the definition of $\tau(\rho)=\int \ell_\rho(\mu,\mu)d^*\mu$ and $\mu d^*\mu = d\mu$.

(iii) For the computation of the integral (32) we note that, in its domain of integration *i.e.* the positive quadrant, the term $P(1/y)-P(x)$ vanishes except in the subset $\Delta\cup\Sigma$ where

$$\Delta := \{(x,y)\mid 0\leqslant x\leqslant 1,\ 0\leqslant y\leqslant 1\}, \qquad \Sigma := \{(x,y)\mid x>1,\ y>1\}.$$

Moreover one has:

$$P(1/y)-P(x) = \begin{cases} 1 & \text{for } (x,y)\in\Delta, \\ -1 & \text{for } (x,y)\in\Sigma. \end{cases}$$

We thus derive

$$\tau(\rho) = 4\rho^{\frac{1}{2}}\left(\int_\Delta \cos(2\pi\rho xy)\cos(2\pi xy)dydx - \int_\Sigma \cos(2\pi\rho xy)\cos(2\pi xy)dydx\right). \tag{35}$$

Let $\alpha(t)$ be the area of the subset $\{(x,y) \in \Delta \mid xy \leqslant t\} \subset \Delta$. For $t < 1$ one has: $\alpha(t) = t + \int_t^1 \frac{t}{x}dx = t - t\log t$. Thus with $I(\Delta) := \int_\Delta \cos(2\pi\rho xy)\cos(2\pi xy)dydx$ one obtains

$$I(\Delta) = \int_0^1 \cos(2\pi\rho t)\cos(2\pi t)d\alpha(t) = \int_0^1 \cos(2\pi\rho t)\cos(2\pi t)(-\log t)dt. \tag{36}$$

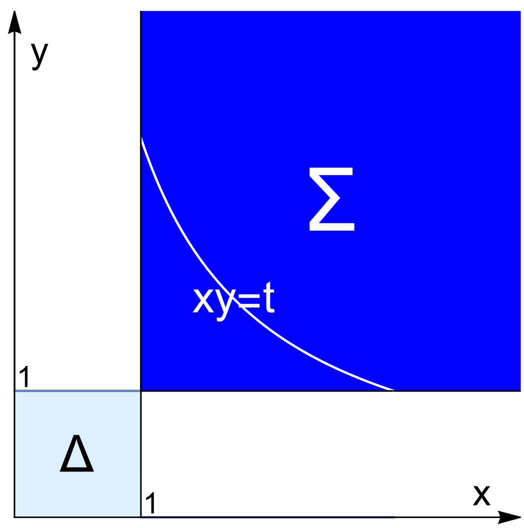

Figure 1. The small square Δ and the big (infinite) square Σ

Let $\beta(t)$ be the area of the subset $\{(x,y) \in \Sigma \mid xy \leqslant t\} \subset \Sigma$. For $t > 1$ one has: $\beta(t) = \int_1^t \frac{t}{x}dx - (t-1) = t\log t - (t-1)$. Thus, with $I(\Sigma) := \int_\Sigma \cos(2\pi\rho xy)\cos(2\pi xy)dydx$, one obtains

$$I(\Sigma) = \int_1^\infty \cos(2\pi\rho t)\cos(2\pi t)d\beta(t) = \int_1^\infty \cos(2\pi\rho t)\cos(2\pi t)\log t dt. \tag{37}$$

This gives in turn

$$\tau(\rho) = 4\rho^{\frac{1}{2}}\left(I(\Delta) - I(\Sigma)\right) = 4\rho^{\frac{1}{2}}\int_0^\infty \cos(2\pi\rho t)\cos(2\pi t)(-\log t)dt \tag{38}$$

that can be rewritten as

$$\tau(\rho) = \rho^{\frac{1}{2}}\int_{\mathbf{R}} \left(\exp(2\pi i(1+\rho)t) + \exp(2\pi i(1-\rho)t)\right)(-\log|t|)dt. \tag{39}$$

The Fourier transform of the distribution $-\log|t|$ is the distribution $W = \mathbf{F}_{e_\mathbf{R}}(-\log|t|) = \frac{1}{2}\frac{1}{|x|}$ (with Weil's normalization). To understand the presence of the factor $\frac{1}{2}$, note that one has the equalities

$$(\mathbf{F}_{e_\mathbf{R}}(\partial_x f))(y) = 2\pi i y(\mathbf{F}_{e_\mathbf{R}}(f))(y), \qquad (\mathbf{F}_{e_\mathbf{R}}(2\pi i x f))(y) = -\partial_y(\mathbf{F}_{e_\mathbf{R}}(f))(y)$$

and hence one obtains

$$(\mathbf{F}_{e_\mathbf{R}}(x\partial_x f))(y) = -\partial_y(y\mathbf{F}_{e_\mathbf{R}}(f))(y).$$

Since $-t\partial_t(-\log|t|) = 1$, the distribution W fulfills the equation $\partial_y(yW) = \underline{\delta}_0$, so that one obtains: $yW = \frac{1}{2}\mathrm{sign}(y)$ (since yW is odd) and $W(y) = \frac{1}{2}\frac{1}{|y|}$. With this definition of the principal value, (39) gives the Weil distribution ([12] Section 4.2)

$$\tau(\rho) = \frac{\rho^{\frac{1}{2}}}{2}\left(\frac{1}{1+\rho} + \frac{1}{|1-\rho|}\right). \tag{40}$$

(iv) Let us show that $\vartheta_{\mathrm{m}}(f)\frac{1}{2}(u_\infty^* đu_\infty)^g$ is of trace class. It is enough, by using the commutativity of $\vartheta_{\mathrm{m}}(f)$ with the bounded operator $(u_\infty^*)^g$, to show that $\vartheta_{\mathrm{m}}(f)\,(đu_\infty)^g$ is of trace class. Using the Fourier transform $\hat f$ and its associated multiplication operator one has

$$\vartheta_{\mathrm{m}}(f)\,(đu_\infty)^g = (\hat f đu_\infty)^g = \left(đ(\hat f u_\infty) - đ(\hat f)u_\infty\right)^g.$$

Thus it suffices to show that for $f \in \mathcal{S}(\mathbf{R}_+^*)$, the function $h = \hat f u_\infty$ is in the Schwartz space $\mathcal{S}(\mathbf{R})$ (see Lemma D.1). To prove this one needs to control the behavior at $\pm\infty$ of the function h. We know that it is of rapid decay since u_∞ is of modulus one. Moreover, one has

$$\partial_s(h) = \partial_s(\hat f)u_\infty + \hat f\partial_s(u_\infty) = \partial_s(\hat f)u_\infty + 2i\hat f u_\infty\partial\theta$$

where θ is the Riemann-Siegel angular function (see (155)) and its derivative $\partial\theta(s)$ is $O(\log|s|)$ when $|s| \to \infty$. Thus $\partial_s(h)$ is of rapid decay. One controls the growth of the higher derivatives of θ by using Binet's first formula

$$\log(\Gamma(z)) = (z-\frac{1}{2})\log z - z + \frac{1}{2}\log(2\pi) + \int_0^\infty\left(\frac{1}{\exp(t)-1} - \frac{1}{t} + \frac{1}{2}\right)e^{-tz}\frac{dt}{t}$$

which, applied at $z = \frac{1}{4} + i\frac{s}{2}$, gives for the first derivative

$$\partial_s\log(\Gamma(\frac{1}{4}+i\frac{s}{2})) = \frac{i}{2}\log\left(\frac{1}{4}+i\frac{s}{2}\right) - \frac{1}{2s-i} - \frac{i}{2}\int_0^\infty\left(\frac{1}{\exp(t)-1} - \frac{1}{t} + \frac{1}{2}\right)e^{-t(\frac{1}{4}+i\frac{s}{2})}dt$$

and shows that all the higher derivatives are bounded. The higher derivatives of h involve sums of products of $\partial_s^k(\hat f)u_\infty$ by products of derivatives of $\partial\theta$. Since the latter are of tempered growth, one concludes that all the higher derivatives $\partial_s^k(h)$ are of rapid decay so that the function h is in $\mathcal{S}(\mathbf{R})$. This shows that $\vartheta_{\mathrm{m}}(f)\frac{1}{2}(u_\infty^* đu_\infty)^g$ is of trace class, its trace is then given by the integral of the diagonal values of its Schwartz kernel which proves (34). □

One checks that (40) is coherent with the equality $W_{\mathbf{R}}(f) = \mathcal{W}_{\mathbf{R}}(\Delta^{-1/2}f)$ (see (151) of Appendix B). The relation between the Mellin transform $\tilde k(z) := \int_0^\infty k(u)u^z d^*u$ and the (multiplicative) Fourier transform $\hat f$ is

$$\tilde k(\frac{1}{2}+is) = \int_0^\infty k(u)u^{\frac{1}{2}+is}d^*u = \int_0^\infty f(u)u^{is}d^*u = \hat f(-s). \tag{41}$$

The negative sign in $-s$ is due to the convention for the multiplicative Fourier transform (22). We specifically note that this direct computation of the trace $\mathrm{Tr}(\hat f\frac{1}{2}u^*đu)$ does not depend on the above normalization (for the sign) since it is done without the use of the multiplicative Fourier transform. What matters is instead the minus sign in front of the distribution $-\log|t|$ in (39). The convention for the multiplicative Fourier transform intervenes twice both in u_∞ and in the operator H defining the quantized calculus and the signs cancel in the expression for $u^*đu$.

2. The square Δ and the trace-remainder

In this section we show that the obstruction to get Weil's positivity at the archimedean place is due to the sole contribution of the small square Δ displayed in Figure 1. We first single out the contribution of Δ by introducing a precise definition of "trace-remainder". We use the same notations of Proposition 1.5 and the definitions of the operators given in (18) and (23). We denote $\vartheta_{\rm m}$ (see (30)) the regular representation of $\mathbf{R}_+^*$ on $L^2(\mathbf{R}_+^*)$. As in (28) of Lemma 1.4, the projection P is the multiplication operator by the characteristic function of $[1,\infty)\subset\mathbf{R}_+^*$.

Definition 2.1 *The trace-remainder is the function of $\rho\in\mathbf{R}_+^*$ given by*

$$\delta(\rho) := \mathrm{Tr}\left(\left(\vartheta_{\rm m}(\rho^{-1}) - P\vartheta_{\rm m}(\rho^{-1})P\right)\frac{1}{2}\,(u_\infty^* \eth u_\infty)^g\right). \tag{42}$$

Next proposition provides an explicit formula for $\delta(\rho)$. In particular it shows that, unlike the distribution $\tau(\rho)$ in (32) (corresponding to $W_{\mathbf{R}}$) that is is not a function because of the divergency at $\rho=1$, $\delta(\rho)$ is a function. Moreover it fulfills the symmetry $\delta(\rho)=\delta(\rho^{-1})$. This fact allows one to extend the explicit formula (valid for $\rho\geqslant 1$) to all of $\mathbf{R}_+^*$. Next equality (44) will play a crucial role in the proof of Corollary 2.3.

Proposition 2.2 *(i) For $\rho\geqslant 1$ one has*

$$\delta(\rho) = 4\rho^{\frac12}\int_\Delta \cos(2\pi\rho xy)\cos(2\pi xy)dydx. \tag{43}$$

(ii) For all $\rho\in\mathbf{R}_+^*$, one has: $\delta(\rho)=\delta(\rho^{-1})$.
(iii) For $f\in C_c(\mathbf{R}_+^*)$, and with $\hat P = (\mathbf{F}^w_{e_{\mathbf{R}}})^{-1}P\mathbf{F}^w_{e_{\mathbf{R}}}$, one has

$$\mathrm{Tr}\left(\vartheta_{\rm m}(f)P\widehat{P}P\right) = \int_0^\infty f(\rho^{-1})\,(\delta(\rho)-\tau(\rho))\,d^*\rho. \tag{44}$$

Proof. (i) For $\rho\in\mathbf{R}_+^*$ and $\xi\in L^2(\mathbf{R}_+^*)$, one has

$$(\vartheta_{\rm m}(\rho^{-1})P\vartheta_{\rm m}(\rho)\xi)(\lambda) = (P\vartheta_{\rm m}(\rho)\xi)(\rho\lambda) = P(\rho\lambda)(\vartheta_{\rm m}(\rho)\xi)(\rho\lambda) = P(\rho\lambda)\xi(\lambda), \qquad \forall\lambda\in\mathbf{R}_+^*.$$

When $\rho\geqslant 1$ one obtains: $P(\lambda)P(\rho\lambda)=P(\lambda)$ for all $\lambda\in\mathbf{R}_+^*$, since both sides are 0 for $\lambda<1$ and 1 for $\lambda\geqslant 1$. Thus, for $\rho\geqslant 1$ one has

$$P\vartheta_{\rm m}(\rho^{-1})P\vartheta_{\rm m}(\rho) = P$$

and so

$$\vartheta_{\rm m}(\rho^{-1}) - P\vartheta_{\rm m}(\rho^{-1})P = \left(1 - P\vartheta_{\rm m}(\rho^{-1})P\vartheta_{\rm m}(\rho)\right)\vartheta_{\rm m}(\rho^{-1}) = (1-P)\vartheta_{\rm m}(\rho^{-1}). \tag{45}$$

By Proposition 1.5, the Schwartz kernel of the operator $(1-P)(\vartheta_{\rm m}(\rho^{-1})\frac12\,(u_\infty^*\eth u_\infty)^g$ is

$$(1-P)(\nu)\ell_\rho(\nu,\mu) = (1-P)(\nu)\ell(\rho\nu,\mu). \tag{46}$$

This equality together with (31) gives the formula

$$(1-P)(\nu)\ell_\rho(\nu,\mu) = 4\rho^{\frac12}\mu^{\frac12}\nu^{\frac12}(1-P)(\nu)\int\cos(2\pi\rho\nu y)\cos(2\pi\mu y)(P(1/y)-P(\mu))dy. \tag{47}$$

Its trace is given by the integral of the diagonal values: $\int(1-P)(\mu)\ell(\rho\mu,\mu)d^*\mu$. This gives, using $\mu d^*\mu = d\mu$, the following expression for $\mu=\nu=x$

$$4\rho^{\frac12}\int_{\substack{x>0\\ y>0}}\cos(2\pi\rho xy)\cos(2\pi xy)(1-P)(x)(P(1/y)-P(x))dydx. \tag{48}$$

Moreover one has: $(1-P)(x)(P(1/y)-P(x)) = (1-P)(x)P(1/y)$ and this product is 0 unless $x<1$ and $y \leqslant 1$, in which case it is equal to 1. Thus (48) reduces to (43).
(ii) The operator $\frac{1}{2}\,(u_\infty^* đu_\infty)^g = (u_\infty^g)^* P u_\infty^g - P$ is self-adjoint. The adjoint of the operator $R(\rho) := \left(\vartheta_{\rm m}(\rho^{-1}) - P\vartheta_{\rm m}(\rho^{-1})P\right)$ is $(\vartheta_{\rm m}(\rho) - P\vartheta_{\rm m}(\rho)P) = R(\rho^{-1})$, thus for any $\rho \in \mathbf{R}_+^*$ one has, using Proposition 1.5 *(iv)* to justify the permutation under the trace

$$\overline{\delta(\rho)} = \mathrm{Tr}\left(\left(R(\rho)\frac{1}{2}\,(u_\infty^* đu_\infty)^g\right)^*\right) = \mathrm{Tr}\left(\frac{1}{2}\,(u_\infty^* đu_\infty)^g R(\rho^{-1})\right) =$$
$$= \mathrm{Tr}\left(R(\rho^{-1})\frac{1}{2}\,(u_\infty^* đu_\infty)^g\right) = \delta(\rho^{-1}).$$

By *(i)*, $\delta(\rho)$ is real for $\rho \geqslant 1$, and the above equality shows that it is real for all $\rho \in \mathbf{R}_+^*$, and that *(ii)* holds.
(iii) One has $\hat{P} = (\mathbf{F}_{e_\mathbf{R}}^w)^{-1} P \mathbf{F}_{e_\mathbf{R}}^w$ and it follows from Lemma 1.3 that $\mathbf{F}_{e_\mathbf{R}}^w = I \circ u_\infty^g$. Thus since $u_\infty^* = u_\infty^{-1}$ one obtains

$$\hat{P} = (u_\infty^{-1})^g \circ I \circ P \circ I \circ u_\infty^g = (u_\infty^*)^g (1-P) u_\infty^g.$$

Using $[P, u_\infty^g] = \frac{1}{2}(đu_\infty)^g$, (see (28)) one gets that the positive operator $P\hat{P}P$ is equal to

$$P\hat{P}P = P(u_\infty^*)^g(1-P)u_\infty^g P = P(u_\infty^*)^g[(1-P), u_\infty^g]P = -P\frac{1}{2}(u_\infty^* đu_\infty)^g P.$$

Thus, working first at the formal level, one obtains for $f \in C_c^\infty(\mathbf{R}_+^*)$

$$\mathrm{Tr}\left(\vartheta_{\rm m}(f)P\hat{P}P\right) = -\mathrm{Tr}\left(\left(\int f(\rho^{-1})\vartheta_{\rm m}(\rho^{-1})d^*\rho\right)P\frac{1}{2}(u_\infty^* đu_\infty)^g P\right) =$$
$$= -\mathrm{Tr}\left(\left(\int f(\rho^{-1})\vartheta_{\rm m}(\rho^{-1})d^*\rho\right)\frac{1}{2}(u_\infty^* đu_\infty)^g\right) +$$
$$+ \int f(\rho^{-1})\mathrm{Tr}\left(\left(\vartheta_{\rm m}(\rho^{-1}) - P\vartheta_{\rm m}(\rho^{-1})P\right)\frac{1}{2}\,(u_\infty^* đu_\infty)^g\right)d^*\rho =$$
$$= \int f(\rho^{-1})\left(\delta(\rho) - \tau(\rho)\right)d^*\rho.$$

One needs to exert care to justify the formal manipulation of replacing

$$\mathrm{Tr}\left(\vartheta_{\rm m}(f)P\frac{1}{2}(u_\infty^* đu_\infty)^g P\right) \quad \text{by} \quad \mathrm{Tr}\left(P\vartheta_{\rm m}(f)P\frac{1}{2}(u_\infty^* đu_\infty)^g\right).$$

In order to justify this step one has to show that $\vartheta_{\rm m}(f)P\frac{1}{2}(u_\infty^* đu_\infty)^g$ is of trace class. For f in the Schwartz space $\mathcal{S}(\mathbf{R}_+^*)$, its (multiplicative) Fourier transform is in $\mathcal{S}(\mathbf{R})$ and thus the commutator $[P, \vartheta_{\rm m}(f)]$ is of trace class. Since $(u_\infty^* đu_\infty)^g$ is bounded, it is thus enough to show that $\vartheta_{\rm m}(f)(u_\infty^* đu_\infty)^g$ is of trace class which follows from Proposition 1.5 *(iv)*. □

It follows from Proposition 2.2 *(i)* and (36), that for $\rho \geqslant 1$, one has

$$\delta(\rho) = 4\rho^{\frac{1}{2}} I(S) = 4\rho^{\frac{1}{2}} \int_0^1 \cos(2\pi\rho t)\cos(2\pi t)(-\log t)dt. \tag{49}$$

One can also check that

$$\int_0^1 \cos(2\pi a t)\,(-\log t)dt = \frac{\mathrm{Si}(2\pi a)}{2\pi a}$$

where $\mathrm{Si}(z)$ is the Sine Integral function $\mathrm{Si}(z) := \int_0^z \frac{\sin(t)}{t}dt$: an entire function of $z \in \mathbf{C}$. Using the formula $2\cos(x)\cos(y) = \cos(x+y) + \cos(x-y)$, one thus obtains, for $\rho \geqslant 1$

$$\delta(\rho) = 2\rho^{\frac{1}{2}}\left(\frac{\mathrm{Si}(2\pi(1+\rho))}{2\pi(1+\rho)} + \frac{\mathrm{Si}(2\pi(\rho-1))}{2\pi(\rho-1)}\right). \tag{50}$$

Near $\rho = 1$, and for $\rho \geqslant 1$, one has the following expansion

$$\delta(\rho) = 2\left(\frac{\mathrm{Si}(4\pi)}{4\pi} + 1\right) + (\rho - 1) - \frac{\left(9\mathrm{Si}(4\pi) + 64\pi^3\right)}{144\pi}(\rho-1)^2 + O\left((\rho-1)^3\right) \tag{51}$$

Since $\delta(\rho) = \delta(\rho^{-1})$ (Proposition 2.2 (ii)), this shows that the function $\delta(\rho)$ has a jump in its first derivative at $\rho = 1$. This fact will play a key role in Chapter 4 (Theorem 3.6).

Since the Sine Integral function $\mathrm{Si}(z)$ is positive for $z \geqslant 0$, $\delta(\rho)$ is positive. Its graph is shown in Figure 2.

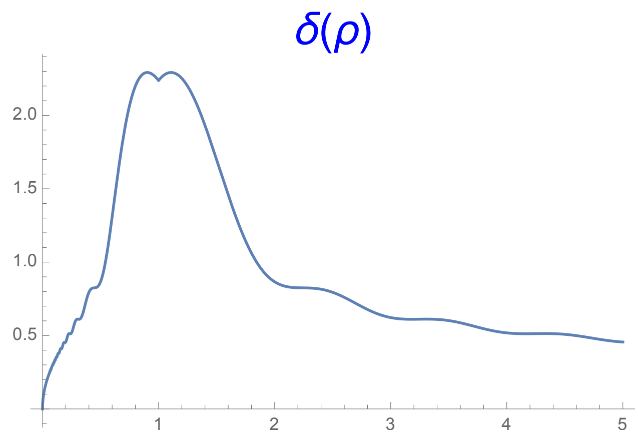

Figure 2. Graph of $\delta(\rho)$

Proposition 2.2 also provides the following corollary which represents a crucial step towards the positivity of $W_\infty = -W_{\mathbf{R}}$, by expressing W_∞ (*i.e.* the functional defined by $-\tau$) as the difference between a positive functional L and the functional defined by δ. In the second statement the positivity of L is translated in terms of Fourier transforms.

Corollary 2.3 (i) *The functional $L = D + W_\infty$ is positive on the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$*

$$L(f) = \int f(\rho^{-1})\left(\delta(\rho) - \tau(\rho)\right) d^*\rho. \tag{52}$$

(ii) *The function $2\theta'(t) + \hat\delta(t)$ is non-negative, where $\hat\delta(t) := \int_{\mathbf{R}_+^*} \delta(\rho)\rho^{-it} d^*\rho$.*

Proof. (i) By Proposition 2.2 (iii) $L(f) := \mathrm{Tr}\left(\vartheta_{\mathrm{m}}(f)P\widehat{P}P\right)$ is positive for $f = g * g^*$ as the trace of a product of two positive operators.
(ii) By applying (164), one has

$$-\int f(\rho^{-1})\tau(\rho)d^*\rho = -\mathrm{Tr}\left(\hat f\left(\frac{1}{2}u^{-1}\bar{d}u\right)\right) = \int \hat f(t)\frac{2\partial_t\theta(t)}{2\pi}dt.$$

Moreover, by Parseval's formula,

$$\int f(\rho^{-1})\delta(\rho)d^*\rho = \int f(\rho)\delta(\rho)d^*\rho = \frac{1}{2\pi}\int \hat f(t)\hat\delta(t)dt.$$

Thus one obtains

$$L(f) = \int \hat{f}(t) \left(2\partial_t \theta(t) + \hat{\delta}(t)\right) \frac{dt}{2\pi} \tag{53}$$

and the positivity of L implies (in fact it is equivalent to) the positivity of the function $2\theta'(t) + \hat{\delta}(t)$. □

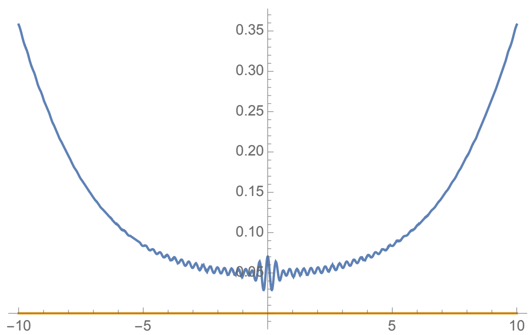

FIGURE 3. Graph of $2\theta'(t)+\hat{\delta}(t)$ in $[-10, 10]$

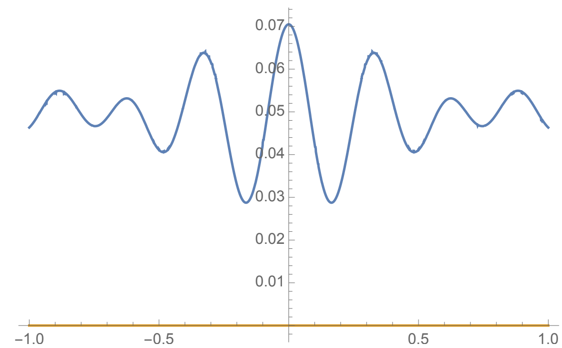

FIGURE 4. Graph of $2\theta'(t) + \hat{\delta}(t)$ in $[-1, 1]$

Figures 3 and 4 show the graph of $2\theta'(t)+\hat{\delta}(t)$ in two versions (the second is zoomed near the origin) displaying that this function is positive. We use the formula (obtained from the symmetry $\delta(\rho) = \delta(\rho^{-1})$)

$$\hat{\delta}(t) = \int_1^\infty \delta(\rho) 2\cos(t \log \rho) d^*\rho.$$

One knows that $\frac{\mathrm{Si}(x)}{x} \leqslant 1$ for $x > 0$, while $\mathrm{Si}(x) \leqslant 2$ for $x > 0$ and $\mathrm{Si}(x) \to \pi/2$ as $x \to \infty$. This provides the estimate, as $\rho \to \infty$,

$$\delta(\rho) = \rho^{-1/2} + O\left(\rho^{-3/2}\right)$$

showing that the function $\hat{\delta}(t)$ is smooth since the derivatives in t only involve powers of $\log \rho$ which do not alter the absolute convergence of the integral.

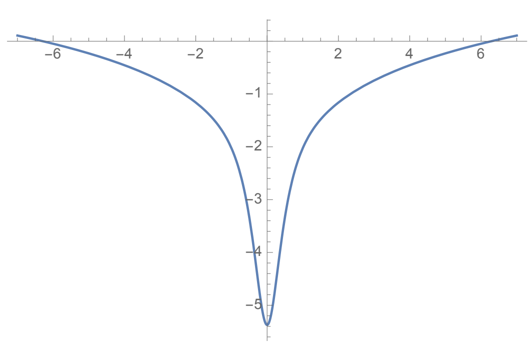

FIGURE 5. Graph of $2\theta'(t)$ in $[-7, 7]$

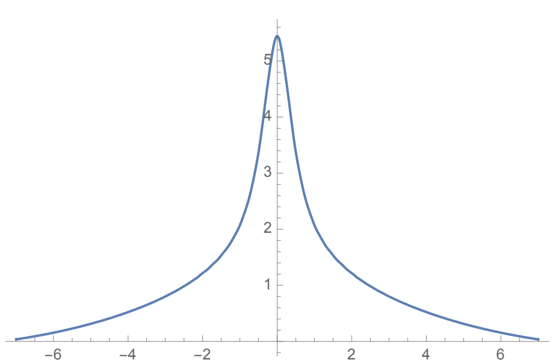

FIGURE 6. Graph of $\hat{\delta}(t)$ in $[-7, 7]$

The graphs in Figures 5 and 6 show the striking precision with which $\hat{\delta}(t)$ imitates the function $-2\theta'(t)$ in the interval $[-7, 7]$. However, unlike $2\theta'(t)$ which tends to infinity when $|t| \to \infty$, the function $\hat{\delta}(t)$ tends to 0 when $|t| \to \infty$, being the Fourier transform of an integrable function.

3. Support and boundary conditions

Throughout this section we use the following terminology

Definition 3.1 *Let G be a locally compact abelian group and $f \in L^1(G, dg)$. We say that f is positive definite when its Fourier transform is pointwise positive, i.e. $\widehat{f}(t) \geqslant 0$, $\forall t \in \widehat{G}$.*

We recall the following result of Boas and Kac ([5] Lemma 5.1 and [22] applied to the multiplicative group $\mathbf{R}_+^*$ (isomorphic to $\mathbf{R}$))

Proposition 3.2 *Let $f \in C_c^\infty(\mathbf{R}_+^*)$ have support in the interval $I = [\lambda^{-1}, \lambda] \subset \mathbf{R}_+^*$. The following conditions are equivalent*

(i) *The Fourier transform $\widehat{f}$ is pointwise positive.*

(ii) *There exists $g \in C_c^\infty(\mathbf{R}_+^*)$ with support in $\sqrt{I} = [\lambda^{-1/2}, \lambda^{1/2}]$ such that $f = g * g^*$.*

Proof. Assume 1. Then by Lemma 5.1 of [5] (the Fourier transform of f is in $L^1(\mathbf{R})$ and is pointwise positive) f can be written as $g * g^*$, where g is square integrable and has support in $\sqrt{I}$. One has $\widehat{f}(t) = |\widehat{g}(t)|^2$, and since $f \in C_c^\infty(\mathbf{R}_+^*)$, one gets $\widehat{f}(t) = O(|t|^{-N})$ for any N. The same holds for $\widehat{g}(t)$ showing that g is smooth.
Conversely, the equality $\widehat{f}(t) = |\widehat{g}(t)|^2$ shows that f is positive definite, moreover its support is contained in I. □

Next, we investigate the following functional on the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$

$$W_\infty(f) = -\int f(\rho^{-1})\tau(\rho)d^*\rho \tag{54}$$

for test functions f whose support is in the interval $[\frac{1}{2}, 2]$. For any complex number t the functional

$$\Phi_t(f) := \widehat{f}(t) = \int f(\rho)\rho^{-it}d^*\rho$$

defines a character of the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$. We assume the vanishing conditions

$$\int f(\rho)\rho^{\pm\frac{1}{2}}d^*\rho = 0 \tag{55}$$

to isolate on the left hand side of the explicit formula the contribution of the zeros of the Riemann zeta function. Next lemma shows that, in the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$, the ideal $\mathcal{J}$ defined by the vanishing condition (55) is the range of a second order differential operator

Lemma 3.3 *(i) The vanishing conditions* (55) *define an ideal $\mathcal{J}$ in the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$.*
(ii) Let $g \in C_c^\infty(\mathbf{R}_+^*)$, then $(-(\rho\partial_\rho)^2 + \frac{1}{4})g \in \mathcal{J}$ and its support is contained in the support of g.
(iii) Let $f \in C_c^\infty(\mathbf{R}_+^*)$ with support in an interval I, fulfill the vanishing conditions (55)*. Then there exists uniquely $g \in C_c^\infty(\mathbf{R}_+^*)$ with support in I and such that*

$$Q(g) := (-(\rho\partial_\rho)^2 + \frac{1}{4})g = f. \tag{56}$$

One has $g = Y^* * Y * f$, where $Y(\rho) = 0$ for $\rho < 1$, $Y(\rho) = \rho^{\frac{1}{2}}$ for $\rho \geqslant 1$ and $Y^*(\rho) := Y(\rho^{-1})$.
(iv) Let f and g as in (iii), then f is positive definite if and only if g is positive definite.

Proof. (*i*) One has $\mathcal{J} = \ker \Phi_{i/2} \cap \ker \Phi_{-i/2}$.
(*ii*) Notice that the (linear) kernel of the operator $-(\rho\partial_\rho)^2 + \frac{1}{4}$ acting on distributions[8] on $\mathbf{R}_+^*$ contains the functions $\rho^{\pm\frac{1}{2}}$. Using integration by parts, since g has compact support, one gets

$$\int \left((-(\rho\partial_\rho)^2 + \frac{1}{4})g(\rho) \right) \rho^{\pm\frac{1}{2}} d^*\rho = \int g(\rho) \left((-(\rho\partial_\rho)^2 + \frac{1}{4})\rho^{\pm\frac{1}{2}} \right) d^*\rho = 0.$$

Moreover $(-(\rho\partial_\rho)^2 + \frac{1}{4})g(\rho)$ vanishes identically outside the support of g.
(*iii*) The kernel of Q in $C_c^\infty(\mathbf{R}_+^*)$ is trivial. The vanishing conditions (55) give $\int_I v^{-\frac{1}{2}} f(v)\, d^*v = 0$ and this shows that the function $k(u) := u^{\frac{1}{2}} \int_0^u v^{-\frac{1}{2}} f(v)\, d^*v$ vanishes when $u \notin I$. Thus the support of k is contained in I. Using again integration by parts and (55) one obtains

$$\int_I u^{\frac{1}{2}} k(u) d^*u = \int_I \left(\int_0^u v^{-\frac{3}{2}} f(v)\, dv \right) du = -\int_I u^{-\frac{3}{2}} f(u) u du = -\int_I u^{\frac{1}{2}} f(u) d^*u = 0.$$

Thus one again derives that $g(\rho) := \rho^{-\frac{1}{2}} \int_\rho^\infty u^{\frac{1}{2}} k(u) d^*u$ also has support in I. Moreover, one has

$$\begin{aligned}
\rho\partial_\rho g(\rho) &= -\frac{1}{2} g(\rho) - \rho^{-\frac{1}{2}} \rho \int_0^\rho v^{-\frac{1}{2}} f(v)\, d^*v, \\
(\rho\partial_\rho)^2 g(\rho) &= -\frac{1}{2} \rho\partial_\rho g(\rho) - \rho\partial_\rho \left(\rho^{\frac{1}{2}} \int_0^\rho v^{-\frac{1}{2}} f(v)\, d^*v \right) = \\
&= -\frac{1}{2} \rho\partial_\rho g(\rho) - \frac{1}{2} \left(\rho^{\frac{1}{2}} \int_0^\rho v^{-\frac{1}{2}} f(v)\, d^*v \right) - f(\rho) = \frac{1}{4} g(\rho) - f(\rho).
\end{aligned}$$

This gives $Q(g) = (-(\rho\partial_\rho)^2 + \frac{1}{4})g = f$. Note that by construction one has: $k = Y * f$, where $Y(\rho) = 0$ for $\rho < 1$ and $Y(\rho) = \rho^{\frac{1}{2}}$ for $\rho \geqslant 1$ and that $g = Y^* * Y * f$.
(*iv*) follows since the Fourier transforms of g and f are related by the equality $(\frac{1}{4} + t^2)\widehat{g}(t) = \widehat{f}(t)$. ☐

Definition 3.4 *Let $E \subset C_c^\infty(\mathbf{R}_+^*)$ be a subspace and $\mathcal{L}$ a linear form on E. Then $\mathcal{L}$ is said to be positive if $\mathcal{L}(f) \geqslant 0$ for any positive definite $f \in E$.*

Next proposition plays a central role. It gives a criterion to test the positivity of a functional ϕ after imposing the vanishing conditions (55), *i.e.* on the intersection $C_c^\infty(I) \cap \mathcal{J}$, by testing the positivity of $\phi \circ Q$ under the same support conditions *i.e.* on $C_c^\infty(I)$.

Proposition 3.5 *Let ϕ be a functional on $C_c^\infty(\mathbf{R}_+^*)$ and I a symmetric interval. Then the restriction of ϕ to $C_c^\infty(I) \cap \mathcal{J}$ is positive if and only if the functional $\phi \circ Q$ is positive on $C_c^\infty(I) \subset C_c^\infty(\mathbf{R}_+^*)$.*

Proof. Assume that the restriction of ϕ to $C_c^\infty(I) \cap \mathcal{J}$ is positive and let $g \in C_c^\infty(I)$ be positive definite. Then Qg is also positive definite by Lemma 3.3 (*iv*). Moreover by (*i*) of the same lemma one has: $Qg \in C_c^\infty(I) \cap \mathcal{J}$. Thus $\phi(Qg) \geqslant 0$.
Conversely, assume that the functional $\phi \circ Q$ is positive on $C_c^\infty(I) \subset C_c^\infty(\mathbf{R}_+^*)$ and let $f \in C_c^\infty(I) \cap \mathcal{J}$ be positive definite. Let $g \in C_c^\infty(I) \subset C_c^\infty(\mathbf{R}_+^*)$, with $Qg = f$ (Lemma 3.3 (*iii*)), then by (*iv*) of the same lemma, g is positive definite so that $\phi(f) = \phi(Qg) \geqslant 0$. ☐

[8] *i.e.* here the dual of $C_c^\infty(\mathbf{R}_+^*)$ which is strictly larger than the space $\mathcal{S}'(\mathbf{R}_+^*)$ of tempered distributions, and $\rho^{\pm\frac{1}{2}} \notin \mathcal{S}'(\mathbf{R}_+^*)$

As just proved in the proposition, for a given functional $\phi \in C_c^\infty(\mathbf{R}_+^*)$ the positivity of ϕ on $C_c^\infty(I)$ implies the positivity of $\phi \circ Q$ on $C_c^\infty(I)$. Next, we explain why it is easier to obtain the positivity of $\phi \circ Q$ on $C_c^\infty(I) \subset C_c^\infty(\mathbf{R}_+^*)$ than the positivity of ϕ (on $C_c^\infty(I)$).

Consider the functional

$$D(f) = \int f(\rho^{-1})\delta(\rho)d^*\rho. \tag{57}$$

It follows from Corollary 2.3 that the functional $L = D + W_\infty$, with W_∞ as in (54), is positive on $C_c^\infty(\mathbf{R}_+^*)$. One derives from Proposition 3.5 the following implication

$$D \circ Q \leqslant 0 \;\text{ on }\; C_c^\infty(I) \implies W_\infty \geqslant 0 \;\text{ on }\; C_c^\infty(I) \cap \mathcal{J}. \tag{58}$$

Next theorem shows that the quadratic form $D \circ Q(\xi * \xi^*)$ associated to $D \circ Q$ is essentially negative. Therefore one needs to impose only finitely many linear conditions on test functions to obtain $D \circ Q \leqslant 0$ and hence $W_\infty \geqslant 0$ on $C_c^\infty(I) \cap \mathcal{J}$.

Theorem 3.6 *Let $I \subset \mathbf{R}_+^*$ be a symmetric and bounded interval. There exists a compact operator K_I in the Hilbert space $L^2(\sqrt{I}, d^*\rho)$ such that for any vector $\xi \in L^2(\sqrt{I}, d^*\rho)$ one has*[9]

$$D \circ Q(\xi * \xi^*) = \langle \xi \mid (-2\,Id + K_I)\xi \rangle = -2\|\xi\|^2 + \langle \xi \mid K_I\,\xi \rangle. \tag{59}$$

Proof. We use the group isomorphism $\exp : \mathbf{R} \to \mathbf{R}_+^*$ to transfer the statement to the convolution algebra $C_c^\infty(\mathbf{R})$ and the interval $I' := \log I$. The operator Q becomes

$$Q_+ := -\partial_x^2 + \frac{1}{4}$$

and the intent is to analyse the functional $D_+ \circ Q_+$ on $C_c^\infty(I') \subset C_c^\infty(\mathbf{R})$ where

$$D_+(f) := \int f(x)\delta(\exp(|x|))dx, \qquad \forall f \in C_c^\infty(\mathbf{R}).$$

We use the symmetry $\delta(\rho) = \delta(\rho^{-1})$ to reformulate the integrand. Using integration by parts one obtains

$$D_+(Q_+f) = \int Q_+f(x)\delta(\exp(|x|))dx = \int f(x)Q_+\delta(\exp(|x|))dx$$

where $Q_+\delta(\exp(|x|))$ is a distribution. One has

$$\delta(\exp(|x|)) = 2\left(\frac{\mathrm{Si}(4\pi)}{4\pi} + 1\right) + |x| + \frac{\left(-9\mathrm{Si}(4\pi) - 64\pi^3 + 72\pi\right)x^2}{144\pi} + O\left(|x|^3\right).$$

Thus $Q_+\delta(\exp(|x|)) = (-\partial_x^2 + \frac{1}{4})\delta(\exp(|x|))$ gives the sum of $-2\underline{\delta}_0$ (where $\underline{\delta}_0$ is the Dirac distribution at 0) and the even function which coincides with $(-\partial_x^2 + \frac{1}{4})\delta(\exp(x))$ for $x \geqslant 0$. Equivalently, one has

$$D_+(Q_+f) = -2f(0) + \int_0^\infty (f(x) + f(-x))Q_+\delta(\exp(x))dx. \tag{60}$$

Now we let $f = \xi * \xi^*$, where $\xi \in L^2(\sqrt{I}, d^*\rho)$. Then: $f(0) = (\xi * \xi^*)(0) = \|\xi\|^2$. The following formula defines a compact operator K_I in the Hilbert space $L^2(\sqrt{I}, d^*\rho)$

$$\langle \xi \mid K_I(\eta) \rangle := \int_1^\infty \left((\xi^* * \eta)(\rho) + (\xi^* * \eta)(\rho^{-1})\right) Q\delta(\rho)d^*\rho,$$

[9] We use the convention that the inner product $\langle \xi \mid \eta \rangle$ is antilinear in ξ (and linear in η)

which gives (59), using (60). To prove that K_I is a compact operator we first show that it is given by a Schwartz kernel $\tilde{K}_I(v,u)$. One has

$$(\xi^* * \eta)(\rho) = \int \overline{\xi(u^{-1})}\eta(\rho u^{-1})d^*u, \quad \int_1^\infty (\xi^* * \eta)(\rho)Q\delta(\rho)d^*\rho = \int_J \overline{\xi(v)}\eta(u)Q\delta(u/v)d^*ud^*v$$

where $J = \{(v,u) \in \sqrt{I} \times \sqrt{I} \mid u/v \geqslant 1\}$. Similarly one gets

$$(\xi^* * \eta)(\rho^{-1}) = \int \overline{\xi(u^{-1})}\eta(\rho^{-1}u^{-1})d^*u,$$

$$\int_1^\infty (\xi^* * \eta)(\rho^{-1})Q\delta(\rho)d^*\rho = \int_{J'} \overline{\xi(v)}\eta(u)Q\delta(v/u)d^*ud^*v$$

where $J' = \{(v,u) \in \sqrt{I} \times \sqrt{I} \mid v/u \geqslant 1\}$. This shows that the Schwartz kernel $\tilde{K}_I(v,u)$ is defined as follows

$$\tilde{K}_I(v,u) = \begin{cases} Q\delta(u/v) & \text{if } u \geqslant v, \\ Q\delta(v/u) & \text{if } v \geqslant u. \end{cases}$$

Since the interval $\sqrt{I}$ is bounded, the function $\tilde{K}_I(v,u)$ is square integrable and hence the operator K_I is of Hilbert-Schmidt class and hence compact. □

4. Moving Δ inside Σ

In the previous section we proved that the functional $D(f) = \int f(\rho^{-1})\delta(\rho)d^*\rho$ is the difference $L - W_\infty$ of the positive functional L in (52) and the Weil functional W_∞ (54). The implication (58) shows that in order to prove Weil's positivity one needs to control the sign of the functional $D \circ Q$, where the differential operator $Q = -(\rho\partial_\rho)^2 + \frac{1}{4}$ implements the vanishing conditions (55) (Proposition 3.5). Moreover, in Theorem 3.6 we proved that the functional $D \circ Q$ is essentially negative since it is represented by the operator $-2\,\mathrm{Id} + K_I$, where K_I is a compact operator depending on the interval I on which the test functions are supported.

In this section we refine the decomposition $W_\infty = L - D$ (Theorem 4.6) in the form: $W_\infty = S - E$, where $S < L$ is still a positive trace-functional, and the negativity of the "remainder" E, will be easier to handle (later in the paper) since $E < D$. This refinement plays a crucial role in the explicit computations of Section 6.

The main idea is to implement the geometry of pairs of projections in Hilbert space to "move" the contribution of the small square Δ inside the big square Σ.

The starting point is the following Lemma 4.1 which allows one to relate the trace $\delta(\rho)$ of (42) with the cutoff projections introduced in [11]. Here, as above, P denotes the projection operator given in $L^2(\mathbf{R}_+^*, d^*\lambda)$ as multiplication by the characteristic function $1_{[1,\infty)}$ and $\widehat{P} = (\mathbf{F}_{e_\mathbf{R}}^w)^{-1}P\mathbf{F}_{e_\mathbf{R}}^w$.

Lemma 4.1 *For $\rho \geqslant 1$ one has*

$$\delta(\rho) = \mathrm{Tr}\left(\vartheta_\mathrm{m}(\rho^{-1})(1-\widehat{P})\,(1-P)\right). \tag{61}$$

Proof. Since $\rho \geqslant 1$ it follows from (45) that

$$\vartheta_\mathrm{m}(\rho^{-1}) - P\vartheta_\mathrm{m}(\rho^{-1})P = (1-P)\vartheta_\mathrm{m}(\rho^{-1})$$

so that one obtains

$$\delta(\rho) = \mathrm{Tr}\left(\left(\vartheta_{\rm m}(\rho^{-1}) - P\vartheta_{\rm m}(\rho^{-1})P\right)\frac{1}{2}\,(u_\infty^* đu_\infty)^g\right) = \mathrm{Tr}\left((1-P)\vartheta_{\rm m}(\rho^{-1})\frac{1}{2}\,(u_\infty^* đu_\infty)^g\right) =$$

$$= \mathrm{Tr}\left((1-P)\vartheta_{\rm m}(\rho^{-1})\left((u_\infty^g)^*\,P\,u_\infty^g - P\right)\right).$$

Now we use the equalities $\mathbf{F}_{e_{\mathbf{R}}}^w = I \circ u_\infty^g$ (see (25)) and $I \circ P \circ I = 1 - P$ and get

$$(u_\infty^g)^*\,P\,u_\infty^g = (\mathbf{F}_{e_{\mathbf{R}}}^w)^{-1}(1-P)\mathbf{F}_{e_{\mathbf{R}}}^w = (1-\widehat{P}).$$

Using the cyclic property of the trace together with $P(1-P) = 0$ we finally have

$$\delta(\rho) = \mathrm{Tr}\left((1-P)\vartheta_{\rm m}(\rho^{-1})\left((u_\infty^g)^*\,P\,u_\infty^g - P\right)\right) = \mathrm{Tr}\left(\vartheta_{\rm m}(\rho^{-1})(1-\widehat{P})\,(1-P)\right).$$

We thus obtain (61). □

Next, we relate in (63) the two projections $1-P$, $1-\widehat{P}$ with the pair $\mathcal{P}_\Lambda$ and $\widehat{\mathcal{P}}_\Lambda$, associated to the cutoff parameter Λ of [11] (see also [12] Chapter 2, §3.3), for $\Lambda = 1$.

We switch to the Hilbert space $L^2(\mathbf{R})_{\rm ev}$ and use the isomorphism w of (17) to rewrite (61) in $L^2(\mathbf{R})_{\rm ev}$. Let $\vartheta := w^{-1}\vartheta_{\rm m}w$ be the unitary representation $\vartheta_{\rm m}$ conjugated by the isomorphism w, its action is given by

$$(\vartheta(\lambda)\,\xi)(v) := \lambda^{-1/2}\,\xi(\lambda^{-1}\,v), \qquad \forall \xi \in L^2(\mathbf{R})_{\rm ev}\,. \tag{62}$$

The projection P (still denoted by the same letter), becomes the multiplication by the characteristic function of the interval complement $\{x \in \mathbf{R} \mid |x| \geqslant 1\}$ while $\widehat{P}$ becomes $\mathbf{F}_{e_{\mathbf{R}}}^{-1}P\mathbf{F}_{e_{\mathbf{R}}}$. These projections are related to the projections $\mathcal{P}_\Lambda$ and $\widehat{\mathcal{P}}_\Lambda$, by the equalities

$$P = 1 - \mathcal{P}_1, \quad \widehat{P} = 1 - \widehat{\mathcal{P}}_1. \tag{63}$$

By implementing these notations Lemma 4.1 states, for $\rho \geqslant 1$ that

$$\delta(\rho) = \mathrm{Tr}\left(\vartheta(\rho^{-1})\widehat{\mathcal{P}}_1\,\mathcal{P}_1\right). \tag{64}$$

We recall the results explained in *op.cit.* to understand the pair of projections $\widehat{\mathcal{P}}_1$, $\mathcal{P}_1$: we refer to *op.cit.* for the proof (the generalities on pairs of projections in Hilbert space follow from Lemma 2.3 of [12]). Giving a pair of orthogonal projections P_i, $i = 1,2$ on a Hilbert space $\mathcal{H}$ is equivalent to giving a unitary representation of the dihedral group $\Gamma = \mathbf{Z}/2\mathbf{Z} * \mathbf{Z}/2\mathbf{Z}$ (the free product of two copies of the group $\mathbf{Z}/2\mathbf{Z}$). One sends the generators to

$$\mathcal{U}_1 = 1 - 2P_1, \qquad \mathcal{U}_2 = 1 - 2P_2$$

and the irreducible representations are at most two dimensional. There exists a unique operator α, $0 \leqslant \alpha \leqslant \pi/2$, commuting with P_i, $i = 1,2$ such that

$$\sin(\alpha) = |P_1 - P_2|. \tag{65}$$

Moreover one has

$$P_1\,P_2\,P_1 = \cos^2(\alpha)P_1\,. \tag{66}$$

Definition 4.2 *The operator α uniquely defined by* (65) *is called the angle operator between P_1 and P_2 and denoted: $\angle(P_1, P_2)$.*

As discovered by D. Slepian and H. Pollack [30, 28] there is a second-order differential operator $\mathbf{W}$ on $\mathbf{R}$, which commutes with both $\mathcal{P}_1$ and $\widehat{\mathcal{P}}_1$: it is defined by

$$(\mathbf{W}\xi)(x) = -\partial((1-x^2)\partial)\,\xi(x) + (2\pi x)^2\,\xi(x). \tag{67}$$

The operator $\mathbf{W}$ commutes with the Fourier transform $\mathbf{F}_{e_\mathbf{R}}$ since

$$(\mathbf{F}_{e_\mathbf{R}}^{-1}\partial\mathbf{F}_{e_\mathbf{R}}\xi)(x) = -2\pi i x\xi(x), \quad \left(-\partial^2 + \mathbf{F}_{e_\mathbf{R}}^{-1}(-\partial^2)\mathbf{F}_{e_\mathbf{R}}\right)\xi(x) = -\partial^2\xi(x) + (2\pi x)^2\,\xi(x).$$

The angle operator $\alpha = \angle(\mathcal{P}_1, \widehat{\mathcal{P}}_1)$ fulfills the equation

$$\mathcal{P}_1\,\widehat{\mathcal{P}}_1\,\mathcal{P}_1 = \cos^2(\alpha)\mathcal{P}_1\,. \tag{68}$$

The eigenfunctions of α are determined using the prolate spheroidal wave functions $PS_{2n,0}(2\pi, x)$ with bandwidth parameter $c = 2\pi$: these are even functions (*i.e.* the integer index $2n$ is even in the traditional notation). They give eigenvectors for the truncated Fourier transform according to the equality (see [28, 29, 30, 26, 33, 34])

$$\int_{-1}^{1} PS_{2n,0}(2\pi, x)\exp(i2\pi x\omega)dx = \lambda(n)PS_{2n,0}(2\pi, \omega). \tag{69}$$

The eigenvalues $\lambda(n)$ are the λ_{2n}^c $(c = 2\pi)$ in the notations of [33]. They are given numerically by the list

$$\lambda(0) = 0.999971,\ \lambda(1) = -0.979485,\ \lambda(2) = 0.524086,\ \lambda(3) = -0.0589766,$$

$$\lambda(4) = 0.00273233,\ \lambda(5) = -0.0000762914, \ldots$$

and all the further ones decay very fast to 0 (see (72)). The equality (69) means that, using the restriction ϕ_n of $PS_{2n,0}(2\pi, x)$ to $[-1, 1]$ as an element of $\mathcal{P}_1 L^2(\mathbf{R})_{\rm ev}$, one has

$$\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\mathcal{P}_1\phi_n = \lambda(n)\mathcal{P}_1\phi_n. \tag{70}$$

In $L^2(\mathbf{R})_{\rm ev}$ the Fourier transform $\mathbf{F}_{e_\mathbf{R}}$ is its own inverse so that $\widehat{\mathcal{P}}_1 = \mathbf{F}_{e_\mathbf{R}}^{-1}\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}} = \mathbf{F}_{e_\mathbf{R}}\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}$. Thus by (70) one gets: $\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\mathcal{P}_1\phi_n = \lambda(n)^2\mathcal{P}_1\phi_n$ and

$$\mathcal{P}_1\widehat{\mathcal{P}_1}\mathcal{P}_1\phi_n = \lambda(n)^2\mathcal{P}_1\phi_n. \tag{71}$$

By construction of the angle operator $\alpha = \angle(\mathcal{P}_1, \widehat{\mathcal{P}}_1)$ one has (68), thus it follows from (71) that the non-zero eigenvalues $\alpha(n)$ of α are given by: $\cos\alpha(n) = |\lambda(n)|$. The sequence $|\lambda(n)|$ is of rapid decay, and one has more precisely the inequality (see [26], Theorem 14, and Appendix F)

$$|\lambda(n)| \leqslant \frac{2^{2n}\pi^{2n+\frac{1}{2}}((2n)!)^2}{(4n)!\Gamma\left(2n+\frac{3}{2}\right)} \sim (4n+1)^{-2n-\frac{1}{2}}(e\pi)^{2n+\frac{1}{2}}. \tag{72}$$

Note that (68) does not determine α on the orthogonal complement of the linear span of the ranges of $\mathcal{P}_1$ and $\widehat{\mathcal{P}}_1$. On this subspace, which is Sonin's space $S(1, 1)$ of Definition 4.3, both $\mathcal{P}_1$ and $\widehat{\mathcal{P}}_1$ are $= 0$ and thus by (65) one has $\angle(\mathcal{P}_1, \widehat{\mathcal{P}}_1)|_{S(1,1)} = 0$.

Definition 4.3 *For $\alpha, \beta > 0$, let Sonin's space $S(\alpha, \beta) \subset L^2(\mathbf{R})_{\rm ev}$ be defined by*

$$S(\alpha, \beta) := \{\xi \in L^2(\mathbf{R})_{\rm ev} \mid \xi(q) = 0,\ \forall q, |q| \leqslant \alpha,\ (\mathbf{F}_{e_\mathbf{R}}\xi)(p) = 0,\ \forall p, |p| \leqslant \beta\}. \tag{73}$$

Given two vectors $\xi, \eta \in \mathcal{H}$ in a Hilbert space $\mathcal{H}$ we shall use the Dirac notation $|\xi\rangle\langle\eta|$ for the rank one projection

$$|\xi\rangle\langle\eta|(\eta') := \xi\,\langle\eta \mid \eta'\rangle, \qquad \forall\eta' \in \mathcal{H}, \tag{74}$$

where by convention the inner product $\langle\eta \mid \eta'\rangle$ is anti-linear in the first vector and linear in η'.

Proposition 4.4 *(i) Let* $\xi_n = \mathcal{P}_1\phi_n/\|\mathcal{P}_1\phi_n\|$, $\eta_n = \mathbf{F}_{e_\mathbf{R}}\xi_n$ *and* $\psi_n = P\eta_n$. *One has*

$$\mathcal{P}_1\eta_n = \mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\xi_n = \lambda(n)\xi_n. \tag{75}$$

(ii) For $\rho \geqslant 1$

$$\delta(\rho) = \mathrm{Tr}\left(\vartheta(\rho^{-1})\widehat{\mathcal{P}}_1\,\mathcal{P}_1\right) = \sum_n \left(\lambda(n)^2\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle + \lambda(n)\langle\xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle\right) \tag{76}$$

(iii) The functions $\psi_n = P\mathbf{F}_{e_\mathbf{R}}\xi_n$ *are real valued, pairwise orthogonal and:* $\|\psi_n\| = \sqrt{1-\lambda(n)^2}$,

$$\sum \lambda(n)^2|\zeta_n\rangle\langle\zeta_n| \leqslant P\widehat{P}P, \qquad \zeta_n = \frac{1}{\sqrt{1-\lambda(n)^2}}\psi_n \tag{77}$$

(iv) Let $\tau(n) := \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}$, *one has*

$$\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = \langle\zeta_n \mid \vartheta(\rho^{-1})\zeta_n\rangle + \tau(n)(\langle\xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle) + \langle\zeta_n \mid \vartheta(\rho^{-1})\xi_n\rangle). \tag{78}$$

Proof. *(i)* This follows from (70).
(ii) The vectors ξ_n form an orthonormal basis of the range of $\mathcal{P}_1$ so that

$$\mathcal{P}_1 = \sum |\xi_n\rangle\langle\xi_n|, \quad \widehat{\mathcal{P}}_1\,\mathcal{P}_1 = \sum |\widehat{\mathcal{P}}_1\xi_n\rangle\langle\xi_n|$$

and, using the equality (70), $\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\mathcal{P}_1\phi_n = \lambda(n)\mathcal{P}_1\phi_n$, one has

$$\widehat{\mathcal{P}}_1\xi_n = \mathbf{F}_{e_\mathbf{R}}\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\xi_n = \lambda(n)\mathbf{F}_{e_\mathbf{R}}\xi_n = \lambda(n)\eta_n \tag{79}$$

which thus gives

$$\widehat{\mathcal{P}}_1\,\mathcal{P}_1 = \sum \lambda(n)|\eta_n\rangle\langle\xi_n|. \tag{80}$$

Hence, using (64) and (80), we obtain

$$\delta(\rho) = \mathrm{Tr}\left(\vartheta(\rho^{-1})\widehat{\mathcal{P}}_1\,\mathcal{P}_1\right) = \sum \lambda(n)\langle\xi_n \mid \vartheta(\rho^{-1})\eta_n\rangle.$$

One has the orthogonal sum: $\eta_n = \mathbf{F}_{e_\mathbf{R}}\xi_n = P\mathbf{F}_{e_\mathbf{R}}\xi_n + \mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\xi_n$ and $\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\xi_n = \lambda(n)\xi_n$. Thus $\eta_n = \psi_n + \lambda(n)\xi_n$ which gives (76) and

$$\widehat{\mathcal{P}}_1\,\mathcal{P}_1 = \sum \lambda(n)^2|\xi_n\rangle\langle\xi_n| + \sum \lambda(n)|\psi_n\rangle\langle\xi_n|. \tag{81}$$

(iii) One has

$$\|P\mathbf{F}_{e_\mathbf{R}}\xi_n\|^2 + \|\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\xi_n\|^2 = \|\mathbf{F}_{e_\mathbf{R}}\xi_n\|^2 = \|\xi_n\|^2 = 1$$

$$\|\psi_n\|^2 = \|P\mathbf{F}_{e_\mathbf{R}}\xi_n\|^2 = 1 - \lambda(n)^2, \quad \|\psi_n\| = \sqrt{1-\lambda(n)^2}.$$

For $n \neq m$ one has, by unitarity of the Fourier transform $\mathbf{F}_{e_\mathbf{R}}$,

$$0 = \langle\mathbf{F}_{e_\mathbf{R}}\xi_n, \mathbf{F}_{e_\mathbf{R}}\xi_m\rangle = \langle\eta_n, \eta_m\rangle = \langle\psi_n + \lambda(n)\xi_n, \psi_m + \lambda(m)\xi_m\rangle = \langle\psi_n, \psi_m\rangle$$

so that the $\zeta_n = \frac{1}{\sqrt{1-\lambda(n)^2}}\psi_n$ form an orthonormal family. By (63), if one replaces the pair of projections $(\mathcal{P}_1, \widehat{\mathcal{P}}_1)$ by the pair $(P, \widehat{P})$ the angle operator remains the same: $\angle(\mathcal{P}_1, \widehat{\mathcal{P}}_1) = \angle(P, \widehat{P})$. Consider the decomposition in two dimensional irreducible representations Π_n. Let E_n be the two dimensional eigenspace associated to Π_n

$$E_n := \{\xi \in L^2(\mathbf{R})_{\mathrm{ev}} \mid |\mathcal{P}_1 - \widehat{\mathcal{P}}_1|(\xi) = \sqrt{1-\lambda(n)^2}\;\;\xi\}.$$

Let us show that $\xi_n \in E_n$. The operator $\mathcal{P}_1\widehat{\mathcal{P}}_1\mathcal{P}_1$ is positive and when restricted to the range of $\mathcal{P}_1$ it has simple spectrum with eigenvalues $\lambda(n)^2$. By (70) the eigenvectors are the ξ_n but the one dimensional space $\mathcal{P}_1 E_n \subset E_n$ is also an eigenspace of the operator $\mathcal{P}_1\widehat{\mathcal{P}}_1\mathcal{P}_1$ for the same eigenvalue $\lambda(n)^2$. Thus one gets

$$\xi_n \in \mathcal{P}_1 E_n \subset E_n.$$

It follows from (79) that

$$\eta_n = \lambda(n)^{-1}\widehat{\mathcal{P}}_1\xi_n \in \widehat{\mathcal{P}}_1 E_n \subset E_n$$

and since $\eta_n = \psi_n + \lambda(n)\xi_n$ we get that $\psi_n \in E_n$. It follows that ζ_n is a normalized eigenvector for the angle operator which gives

$$P\widehat{P}P\zeta_n = \lambda(n)^2 P\zeta_n = \lambda(n)^2\zeta_n.$$

The spectral decomposition of the positive operator $P\widehat{P}P$ is of the form

$$P\widehat{P}P = \sum \lambda(n)^2 |\zeta_n\rangle\langle\zeta_n| + \mathbf{S}. \tag{82}$$

Indeed the last term is the restriction of $P\widehat{P}P$ to the orthogonal complement of the subspace $\oplus_n E_n \subset L^2(\mathbf{R})_{\text{ev}}$. This operator $\mathbf{S}$ is the orthogonal projection on Sonin's space $S(1,1)$ of Definition 4.3. Note that by construction the vectors ξ_n are all orthogonal to $S(1,1)$ and so are $\eta_n = \mathbf{F}_{e_\mathbf{R}}\xi_n$ and $\zeta_n = \frac{1}{\sqrt{1-\lambda(n)^2}}(\eta_n - \lambda(n)\xi_n)$.

(iv) We use $\vartheta(\rho) = \mathbf{F}_{e_\mathbf{R}}^{-1}\vartheta(\rho^{-1})\mathbf{F}_{e_\mathbf{R}}$ and the fact that ξ_n is a real valued function, to get

$$\begin{aligned}\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle &= \langle\vartheta(\rho)\xi_n \mid \xi_n\rangle = \langle\xi_n \mid \vartheta(\rho)\xi_n\rangle = \langle\xi_n \mid \mathbf{F}_{e_\mathbf{R}}^{-1}\vartheta(\rho^{-1})\mathbf{F}_{e_\mathbf{R}}\xi_n\rangle = \langle\eta_n \mid \vartheta(\rho^{-1})\eta_n\rangle = \\ &= \langle(\psi_n + \lambda(n)\xi_n) \mid \vartheta(\rho^{-1})(\psi_n + \lambda(n)\xi_n)\rangle = \lambda(n)^2\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle + \\ &+ \langle\psi_n \mid \vartheta(\rho^{-1})\psi_n\rangle + \langle\lambda(n)\xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle + \langle\psi_n \mid \vartheta(\rho^{-1})\lambda(n)\xi_n\rangle.\end{aligned}$$

Thus one gets

$$(1-\lambda(n)^2)\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = \langle\psi_n \mid \vartheta(\rho^{-1})\psi_n\rangle + \lambda(n)\left(\langle\xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle + \langle\psi_n \mid \vartheta(\rho^{-1})\xi_n\rangle\right)$$

and since $\zeta_n = \frac{1}{\sqrt{1-\lambda(n)^2}}\psi_n$ one obtains, with $\tau(n) := \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}$

$$\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = \langle\zeta_n \mid \vartheta(\rho^{-1})\zeta_n\rangle + \tau(n)(\langle\xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle + \langle\zeta_n \mid \vartheta(\rho^{-1})\xi_n\rangle)$$

which is (78). ∎

Remark 4.5 *(i) Equality (76) implies in particular that $\delta(1) = \sum\lambda(n)^2$, i.e.*

$$2\left(\frac{Si(4\pi)}{4\pi} + 1\right) = \sum\lambda(n)^2$$

and one checks numerically that both sides[10] are ~ 2.237484835. One has, by (75), $\mathcal{P}_1\mathbf{F}_{e_\mathbf{R}}\xi_n = \lambda(n)\xi_n$ which implies that $\psi_n(1) = \mathbf{F}_{e_\mathbf{R}}\xi_n(1) = \lambda(n)\xi_n(1)$. The function $\mathbf{F}_{e_\mathbf{R}}\xi_n$ is smooth, being the Fourier transform of a function with compact support. The derivative, at $\rho = 1^+$, of the function $\sum\lambda(n)\langle\xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle$ which appears in (76), is $\sum\lambda(n)\psi_n(1)\xi_n(1)$. This is thus equal to $\sum\lambda(n)^2\xi_n(1)^2$ which is numerically ~ 2. To prove that it is equal to 2, note that, by (51), the derivative of $\delta(\rho)$ at $\rho = 1^+$ is equal to 1 while the derivative of $\langle\xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle$ is (using ξ instead of ξ_n)

$$\partial_\rho\left(\rho^{1/2}\int_0^{\rho^{-1}}\xi(x)\xi(\rho x)dx\right) = \sqrt{\rho}\left(\int_0^{\frac{1}{\rho}} x\xi(x)\xi'(\rho x)\,dx - \frac{\xi(1)\xi\left(\frac{1}{\rho}\right)}{\rho^2}\right) + \frac{\int_0^{\frac{1}{\rho}}\xi(x)\xi(\rho x)\,dx}{2\sqrt{\rho}}.$$

[10] We are only using the even prolate functions, the sum of squares of eigenvalues including the odd ones is 4.

For $\rho = 1$ this gives, using integration by parts,

$$-\xi(1)^2 + \int_0^1 x\xi(x)\xi'(x)\,dx + \frac{1}{2}\int_0^1 \xi(x)^2\,dx = -\frac{1}{2}\xi(1)^2.$$

It follows that the contribution of the sum $\sum \lambda(n)^2\langle \xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle$ to the derivative at $\rho = 1^+$ is $-\frac{1}{2}\sum \lambda(n)^2\xi_n(1)^2$ so that (76) implies: $\sum \lambda(n)^2\xi_n(1)^2 = 2$.
(ii) Note that for $\rho \geqslant 1$ one has

$$\langle \psi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = 0,\ \langle \zeta_n \mid \vartheta(\rho^{-1})\xi_n\rangle = 0, \tag{83}$$

since $\xi_n(\rho x) = 0$ for $|x| > 1$ so that

$$\langle \psi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = \rho^{1/2}\int \xi_n(\rho x)\psi_n(x)dx = 0.$$

Thus one can rewrite (76) in a more symmetric manner replacing the term $\langle \xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle$ (multiplied by $\lambda(n)$) with the symmetric form (using the fact that the ξ_n, ψ_n are real valued)

$$\langle \xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle + \langle \psi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = \langle \xi_n \mid \vartheta(\rho^{-1})\psi_n\rangle + \langle \xi_n \mid \vartheta(\rho)\psi_n\rangle.$$

This sum is invariant under $\rho \mapsto \rho^{-1}$ so that, after this replacement, (76) is valid for all $\rho \in \mathbf{R}_+^*$.

Next theorem refines the local trace formula (44)

Theorem 4.6 *Let $\mathbf{S}$ be the orthogonal projection of $L^2(\mathbf{R})_{\rm ev}$ on the closed subspace $S(1,1)$. The following functional is positive*

$$\mathrm{Tr}(\vartheta(f)\mathbf{S}) = W_\infty(f) + \int f(\rho^{-1})\epsilon(\rho)d^*\rho, \qquad \forall f \in C_c^\infty(\mathbf{R}_+^*), \tag{84}$$

where W_∞ is as in (54), $\epsilon(\rho)$ is the function of $\rho \in \mathbf{R}_+^*$, with $\epsilon(\rho^{-1}) = \epsilon(\rho)$, which is given, for $\rho \geqslant 1$, by

$$\epsilon(\rho) = \sum \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}\langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle. \tag{85}$$

Proof. By (44) one has, rewriting the formula in $L^2(\mathbf{R})_{\rm ev}$,

$$W_\infty(f) + \int f(\rho^{-1})\delta(\rho)d^*\rho = \mathrm{Tr}\left(\vartheta(f)P\widehat{P}P\right). \tag{86}$$

It follows from (76) that, for $\rho \geqslant 1$, one has

$$\delta(\rho) = \sum\left(\lambda(n)^2\langle \xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle + \lambda(n)\sqrt{1-\lambda(n)^2}\langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle\right). \tag{87}$$

By (78), one has

$$\langle \xi_n \mid \vartheta(\rho^{-1})\xi_n\rangle = \langle \zeta_n \mid \vartheta(\rho^{-1})\zeta_n\rangle + \tau(n)(\langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle) + \langle \zeta_n \mid \vartheta(\rho^{-1})\xi_n\rangle). \tag{88}$$

This gives for $\rho \geqslant 1$, the formula

$$\delta(\rho) = \sum \lambda(n)^2\langle \zeta_n \mid \vartheta(\rho^{-1})\zeta_n\rangle + \sum T_n, \tag{89}$$

where

$$T_n = \lambda(n)\sqrt{1-\lambda(n)^2}\langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle + \lambda(n)^2\tau(n)(\langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n\rangle) + \langle \zeta_n \mid \vartheta(\rho^{-1})\xi_n\rangle).$$

Since $\rho \geqslant 1$ one has, by (83): $\langle \zeta_n \mid \vartheta(\rho^{-1})\xi_n \rangle = 0$. Thus one gets, using[11] $\tau(n) = \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}$

$$T_n = \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}} \langle \xi_n \mid \vartheta(\rho^{-1})\zeta_n \rangle.$$

Thus we obtain, for $\rho \geqslant 1$

$$\delta(\rho) = \sum \lambda(n)^2 \langle \zeta_n \mid \vartheta(\rho^{-1})\zeta_n \rangle + \epsilon(\rho). \tag{90}$$

Since both δ, ϵ and the terms $\langle \zeta_n \mid \vartheta(\rho^{-1})\zeta_n \rangle$ are invariant under $\rho \mapsto \rho^{-1}$, we thus obtain, for any test function $f \in C_c^\infty(\mathbf{R}_+^*)$

$$\int f(\rho^{-1})\delta(\rho)d^*\rho = \int f(\rho^{-1})\epsilon(\rho)d^*\rho + \sum \lambda(n)^2 \langle \zeta_n \mid \vartheta(f)\zeta_n \rangle.$$

Using (86) we conclude that

$$W_\infty(f) + \int f(\rho^{-1})\epsilon(\rho)d^*\rho + \sum \lambda(n)^2 \langle \zeta_n \mid \vartheta(f)\zeta_n \rangle = \mathrm{Tr}\left(\vartheta(f)P\widehat{P}P\right).$$

This gives the required formula (85) provided one proves that

$$\mathrm{Tr}\left(\vartheta(f)P\widehat{P}P\right) = \mathrm{Tr}(\vartheta(f)\mathbf{S}) + \sum \lambda(n)^2 \langle \zeta_n \mid \vartheta(f)\zeta_n \rangle. \tag{91}$$

This final formula follows from the spectral decomposition (82) of the operator $P\widehat{P}P$. □

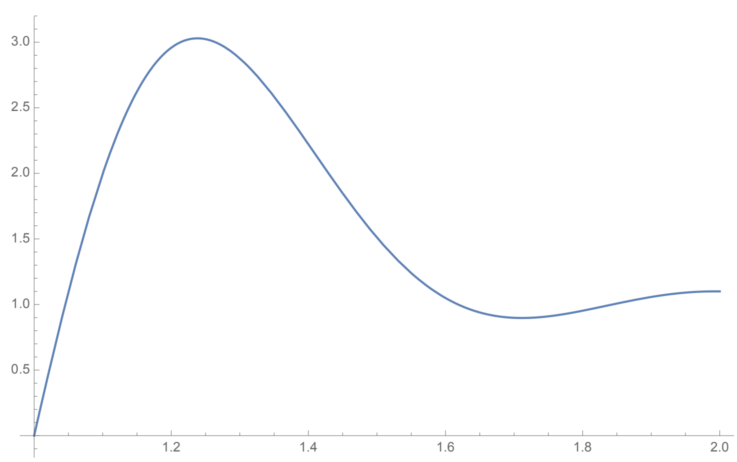

FIGURE 7. Graph of $\epsilon(\rho)$ in $[1, 2]$.

5. The functional $E \circ Q$ and the compact operator $\mathbf{K}_I$

Let E be the functional defined on $C_c^\infty(\mathbf{R}_+^*)$ by

$$E(f) := \int f(\rho^{-1})\epsilon(\rho)d^*\rho, \qquad \forall f \in C_c^\infty(\mathbf{R}_+^*). \tag{92}$$

By Theorem 4.6 the functional $W_\infty + E$ is positive. Thus, to control W_∞ after imposing the vanishing conditions we need, by Proposition 3.5, to analyse the functional $E \circ Q$, with Q as in

[11] Note that for $-1 < \lambda < 1$ one has $\lambda\sqrt{1-\lambda^2} + \lambda^2 \frac{\lambda}{\sqrt{1-\lambda^2}} = \frac{\lambda}{\sqrt{1-\lambda^2}}$

(56). By (85) the function $\epsilon(\rho)$ is a sum of coefficients of the representation of the multiplicative group $\mathbf{R}_+^*$ by scaling. Thus we start by investigating how the operator Q acts on such coefficients. We first assume (Lemma 5.1) that the vectors involved are smooth functions and then compute in Lemma 5.2 the boundary terms in the case of the vectors involved in (85).

The operator $\mathcal{D} := D_u^2 + D_u$, where $D_u(f)x := xf'(x)$ is the scaling Hamiltonian, commutes with the Fourier transform $\mathbf{F}_{e_\mathbf{R}}$ since

$$\mathbf{F}_{e_\mathbf{R}}^{-1} D_u \mathbf{F}_{e_\mathbf{R}} \xi(x) = -\partial_x(x\xi(x)) = ((-1 - D_u)\xi)(x).$$

One has

$$\mathcal{D}(f)(x) = x^2 f''(x) + 2xf'(x) \tag{93}$$

thus $\mathcal{D}(f)(0) = 0$. Since $\mathcal{D}$ commutes with the Fourier transform the range $\mathcal{D}(\mathcal{S}(\mathbf{R}))$ consists of functions fulfilling the two conditions

$$f(0) = \hat{f}(0) = 0. \tag{94}$$

Note also that, for the inner product on $L^2(\mathbf{R})_{\mathrm{ev}}$, the adjoint of D_u is $D_u^*(f)x) := -\partial_x(xf(x))$ and thus $\mathcal{D}^* = \mathcal{D}$.

Lemma 5.1 *Let $\xi, \eta \in L^2(\mathbf{R})_{\mathrm{ev}}$ be smooth functions. Then with Q as in* (56) *and $\mathcal{D} := D_u^2 + D_u$, one has*

$$\langle \eta \mid \vartheta(Qf)\xi \rangle = -\langle \eta \mid \vartheta(f)\mathcal{D}\xi \rangle, \qquad \forall f \in C_c^\infty(\mathbf{R}_+^*). \tag{95}$$

Proof. Using the self-adjointness of Q for the inner product in $L^2(\mathbf{R}_+^*, d^*\rho)$ together with the commutation of Q with the inversion I, one has

$$\langle \eta \mid \vartheta(Qf)\xi \rangle = \int Qf(\rho^{-1}) \langle \eta \mid \vartheta(\rho^{-1})\xi \rangle d^*\rho = \int f(\rho^{-1})(Qk)(\rho) d^*\rho,$$

where the function $k(\rho)$ is defined as

$$k(\rho) := \langle \eta \mid \vartheta(\rho^{-1})\xi \rangle = \rho^{1/2} \int \xi(\rho x)\overline{\eta(x)} dx.$$

To obtain a formula for Qk, we apply Q to the function $g(\rho) := \rho^{1/2}\xi(\rho x)$ and use the equality

$$\rho\partial_\rho \left(\rho^{1/2}\xi(\rho x)\right) = \frac{1}{2}\left(\rho^{1/2}\xi(\rho x)\right) + \rho^{1/2}(D_u\xi)(\rho x)$$

which holds since

$$\rho\partial_\rho\left(\xi(\rho x)\right) = \rho x\, \xi'(\rho x) = (D_u\xi)(\rho x).$$

We thus obtain

$$\begin{aligned}
\rho\partial_\rho\left(\rho\partial_\rho\left(\rho^{1/2}\xi(\rho x)\right)\right) &= \rho\partial_\rho\left(\frac{1}{2}\left(\rho^{1/2}\xi(\rho x)\right)\right) + \rho\partial_\rho\left(\rho^{1/2}(D_u\xi)(\rho x)\right) = \\
&= \frac{1}{4}\left(\rho^{1/2}\xi(\rho x)\right) + \frac{1}{2}\rho^{1/2}(D_u\xi)(\rho x) + \rho\partial_\rho\left(\rho^{1/2}(D_u\xi)(\rho x)\right) = \\
&= \frac{1}{4}\left(\rho^{1/2}\xi(\rho x)\right) + \frac{1}{2}\rho^{1/2}(D_u\xi)(\rho x) + \frac{1}{2}\rho^{1/2}(D_u\xi)(\rho x) + \rho^{1/2}(D_u^2\xi)(\rho x).
\end{aligned}$$

Thus, using (56), we have

$$Qg(\rho) = -(\rho\partial_\rho)^2 g(\rho) + \frac{1}{4}g(\rho) = -\rho^{1/2}(D_u^2\xi)(\rho x) - \rho^{1/2}(D_u\xi)(\rho x) = -\rho^{1/2}(\mathcal{D}\xi)(\rho x).$$

This, in turn, gives

$$Qk(\rho) = -\rho^{1/2} \int (\mathcal{D}\xi)(\rho x)\overline{\eta(x)}dx = -\langle \eta \mid \vartheta(\rho^{-1})(\mathcal{D}\xi)\rangle$$

and

$$\langle \eta \mid \vartheta(Qf)\xi\rangle = \int f(\rho^{-1})(Qk)(\rho)d^*\rho = -\int f(\rho^{-1})\langle \eta \mid \vartheta(\rho^{-1})(\mathcal{D}\xi)\rangle d^*\rho = -\langle \eta \mid \vartheta(f)\mathcal{D}\xi\rangle.$$

which proves (95). ∎

One has $D_u^* = -1 - D_u$, thus $-\mathcal{D} = D_u D_u^* = D_u^* D_u$. Moreover D_u commutes with the scaling action, hence with $\vartheta(f)$, thus one obtains, at the formal level

$$\langle \eta \mid \vartheta(Qf)\xi\rangle = \langle D_u\eta \mid \vartheta(f)D_u\xi\rangle = \langle D_u^*\eta \mid \vartheta(f)D_u^*\xi\rangle. \tag{96}$$

In principle, we would like to apply (96) to (85) and get a formula for $E \circ Q$, but the functions ξ_n and ζ_n do not belong to the domain of the operator D_u, since both have a discontinuity at $x = \pm 1$. This means that some boundary terms appear, and we are going to compute them. Since we handle even functions, we concentrate on the positive real axis and we only consider the scaling parameter $\rho \in [1, 2]$.

Lemma 5.2 *Let $\xi \in C^\infty((0,1])$ and $\zeta \in C^\infty([1,\infty))$ be smooth and real valued functions. Extend first ξ, ζ to $[0,\infty)$ as follows: $\xi(x) := 0$ for $x > 1$ and $\zeta(x) := 0$ for $x < 1$. Then, with Q as in (56) and $k(\rho) = \rho^{1/2}\int_0^\infty \xi(x)\zeta(\rho x)dx$, for $\rho \in (1,2]$, one has*

$$(Qk)(\rho) = \rho^{1/2}\int_{\rho^{-1}}^1 (D_u\xi)(x)(D_u\zeta)(\rho x)dx + \rho^{-1/2}(D_u\xi)(\rho^{-1})\zeta(1) - \rho^{1/2}\xi(1)(D_u\zeta)(\rho). \tag{97}$$

Proof. One has $k(\rho) = \rho^{1/2}\int_{\rho^{-1}}^1 \xi(x)\zeta(\rho x)dx$, since $\xi(x)\zeta(\rho x) = 0$ for $x \notin [\rho^{-1}, 1]$. Furthermore,

$$(\rho\partial_\rho)\left(\rho^{1/2}\int_{\rho^{-1}}^1 \xi(x)\zeta(\rho x)dx\right) = \frac{1}{2}\left(\rho^{1/2}\int_{\rho^{-1}}^1 \xi(x)\zeta(\rho x)dx\right) + \rho^{-1/2}\xi(\rho^{-1})\zeta(1) + \\ + \left(\rho^{1/2}\int_{\rho^{-1}}^1 \xi(x)(D_u\zeta)(\rho x)dx\right),$$

using for the computation of $\rho^{1/2}\rho\partial_\rho\left(\int_{\rho^{-1}}^1 \xi(x)\zeta(\rho x)dx\right)$ the equality

$$\int_{(\rho+\epsilon)^{-1}}^1 \xi(x)\zeta((\rho+\epsilon)x)dx - \int_{\rho^{-1}}^1 \xi(x)\zeta(\rho x)dx = \\ = \int_{(\rho+\epsilon)^{-1}}^{\rho^{-1}} \xi(x)\zeta((\rho+\epsilon)x)dx + \int_{\rho^{-1}}^1 \xi(x)(\zeta((\rho+\epsilon)x) - \zeta(\rho x))dx.$$

By continuity of ζ in $[1,2]$ one has,

$$\frac{1}{\epsilon}\int_{(\rho+\epsilon)^{-1}}^{\rho^{-1}} \xi(x)\zeta((\rho+\epsilon)x)dx \underset{\epsilon\to 0^+}{\longrightarrow} \rho^{-2}\xi(\rho^{-1})\zeta(1).$$

Iterating this formula one obtains, for $k(\rho) = \rho^{1/2}\int_{\rho^{-1}}^1 \xi(x)\zeta(\rho x)dx$

$$(\rho\partial_\rho)^2 k(\rho) = \frac{1}{2}(\rho\partial_\rho)k(\rho) + (\rho\partial_\rho)\left(\rho^{-1/2}\xi(\rho^{-1})\zeta(1)\right) + (\rho\partial_\rho)\left(\rho^{1/2}\int_{\rho^{-1}}^1 \xi(x)(D_u\zeta)(\rho x)dx\right)$$

$$= \frac{1}{4}\left(\rho^{1/2}\int_{\rho^{-1}}^{1}\xi(x)\zeta(\rho x)dx\right) + \frac{1}{2}\rho^{-1/2}\xi(\rho^{-1})\zeta(1) + \frac{1}{2}\left(\rho^{1/2}\int_{\rho^{-1}}^{1}\xi(x)(D_u\zeta)(\rho x)dx\right) +$$

$$+(\rho\partial_\rho)\left(\rho^{-1/2}\xi(\rho^{-1})\zeta(1)\right) + \frac{1}{2}\left(\rho^{1/2}\int_{\rho^{-1}}^{1}\xi(x)(D_u\zeta)(\rho x)dx\right) + \rho^{-1/2}\xi(\rho^{-1})(D_u\zeta)(1)+$$

$$+\left(\rho^{1/2}\int_{\rho^{-1}}^{1}\xi(x)(D_u^2\zeta)(\rho x)dx\right).$$

This gives

$$(Qk)(\rho) = -\rho^{1/2}\int_{\rho^{-1}}^{1}\xi(x)((D_u^2 + D_u)\zeta)(\rho x)dx - B,$$

where the boundary term is

$$B = \frac{1}{2}\rho^{-1/2}\xi(\rho^{-1})\zeta(1) + (\rho\partial_\rho)\left(\rho^{-1/2}\xi(\rho^{-1})\zeta(1)\right) + \rho^{-1/2}\xi(\rho^{-1})(D_u\zeta)(1).$$

Using the equality

$$(\rho\partial_\rho)\left(\rho^{-1/2}\xi(\rho^{-1})\zeta(1)\right) = -\frac{1}{2}\rho^{-1/2}\xi(\rho^{-1})\zeta(1) - \rho^{-3/2}\xi'(\rho^{-1})\zeta(1)$$

one obtains

$$B = \rho^{-1/2}\xi(\rho^{-1})(D_u\zeta)(1) - \rho^{-1/2}(D_u\xi)(\rho^{-1})\zeta(1).$$

The integration by parts, which gives the adjoint of D_u as $-1 - D_u$, is

$$\int_a^b D_u(f)(x)g(x)dx + \int_a^b f(x)((1 + D_u)g)(x)dx = bf(b)g(b) - af(a)g(a)$$

as can be seen by differentiating the product $(xf(x)g(x))' = xf'(x)g(x) + f(x)(g(x) + xg'(x))$. We apply it with $f = \xi$ and $g(x) = D_u\zeta(\rho x)$, and use the commutation of D_u with scaling to get

$$\int_{\rho^{-1}}^{1}(D_u\xi)(x)(D_u\zeta)(\rho x)dx + \int_{\rho^{-1}}^{1}\xi(x)((D_u^2 + D_u)\zeta)(\rho x)dx = \xi(1)(D_u\zeta)(\rho) - \rho^{-1}\xi(\rho^{-1})(D_u\zeta)(1).$$

Hence we obtain

$$(Qk)(\rho) = \rho^{1/2}\int_{\rho^{-1}}^{1}(D_u\xi)(x)(D_u\zeta)(\rho x)dx - \rho^{1/2}\left(\xi(1)(D_u\zeta)(\rho) - \rho^{-1}\xi(\rho^{-1})(D_u\zeta)(1)\right) - B =$$

$$= \rho^{1/2}\int_{\rho^{-1}}^{1}(D_u\xi)(x)(D_u\zeta)(\rho x)dx + \rho^{-1/2}(D_u\xi)(\rho^{-1})\zeta(1) - \rho^{1/2}\xi(1)(D_u\zeta)(\rho).$$

which is the required formula. □

We thus derive the following formula for $Q\epsilon(\rho)$

Proposition 5.3 *For $\rho > 1$ one has the equality*

$$Q\epsilon(\rho) = \sum \frac{\lambda(n)}{\sqrt{1 - \lambda(n)^2}} T_n(\rho), \tag{98}$$

where

$$T_n(\rho) = \rho^{1/2}\int_{\rho^{-1}}^{1}(D_u\xi_n)(x)(D_u\zeta_n)(\rho x)dx + \rho^{-1/2}(D_u\xi_n)(\rho^{-1})\zeta_n(1) - \rho^{1/2}\xi_n(1)(D_u\zeta_n)(\rho) \tag{99}$$

Proof. This follows from (85) combined with Lemma 5.2 and by recalling the normalization (16) of the inner product in $L^2(\mathbf{R})_{\mathrm{ev}}$. We refer to Appendix F for the proof of the convergence of the infinite series and for an explicit control of the remainder. □

When implementing (99) in a computer program, it is convenient to use the function ξ_n^{an} which is the analytic continuation of ξ_n. By (75) one has $\eta_n = \lambda(n)\,\xi_n^{\mathrm{an}}$, thus for $x \in [1,\infty)$, one derives

$$\zeta_n(x) = \frac{1}{\sqrt{1-\lambda(n)^2}}\,\eta_n(x) = \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}\xi_n^{\mathrm{an}}(x).$$

Combining this with Proposition 5.3, one obtains the equality $Q\epsilon(\rho) = \sum \frac{\lambda(n)^2}{1-\lambda(n)^2} C_n$, where

$$C_n = \rho^{1/2}\int_{\rho^{-1}}^{1}(D_u\xi_n^{\mathrm{an}})(x)(D_u\xi_n^{\mathrm{an}})(\rho x)dx + \rho^{-1/2}(D_u\xi_n^{\mathrm{an}})(\rho^{-1})\xi_n^{\mathrm{an}}(1) - \rho^{1/2}\xi_n^{\mathrm{an}}(1)(D_u\xi_n^{\mathrm{an}})(\rho).$$

Using the equality $D_u(f(x) = xf'(x)$ one gets the following formula for C_n

$$C_n = \rho^{1/2}\int_{\rho^{-1}}^{1} x(\xi_n^{\mathrm{an}})'(x)\rho x(\xi_n^{\mathrm{an}})'(\rho x)dx + \rho^{-3/2}(\xi_n^{\mathrm{an}})'(\rho^{-1})\xi_n^{\mathrm{an}}(1) - \rho^{3/2}\xi_n^{\mathrm{an}}(1)(\xi_n^{\mathrm{an}})'(\rho). \quad (100)$$

This formula shows, in particular, that the function $Q\epsilon(\rho)$ is 0 for $\rho = 1$.
Next, we show that the function $\epsilon(\rho)$ which fulfills (85) for $\rho \geqslant 1$, and the symmetry $\epsilon(\rho^{-1}) = \epsilon(\rho)$, has a jump in its derivative at $\rho = 1$, *i.e.* a behavior (at $\rho = 1$) similar to that of the function $\delta(\rho)$.

Lemma 5.4 *The derivative of* $\epsilon(\rho)$ *at* $\rho = 1^+$ *is*

$$\epsilon'(1^+) = \sum \frac{\lambda(n)^2}{1-\lambda(n)^2}\xi_n(1)^2.$$

Proof. By (85), using the above functions ξ_n^{an}, one has

$$\epsilon(\rho) = \sum \frac{\lambda(n)^2}{1-\lambda(n)^2}\left(\rho^{1/2}\int_{\rho^{-1}}^{1}\xi_n^{\mathrm{an}}(x)\xi_n^{\mathrm{an}}(\rho x)dx\right),$$

and moreover $\xi_n^{\mathrm{an}}(1) = \xi_n(1)$. □

The convergence of the series is ensured by the inequality (see [26], Theorem 12)

$$|\xi_n(1)| \leqslant \sqrt{2n+\frac{1}{2}}. \quad (101)$$

The numerical values of the terms $t(n) = \frac{\lambda(n)^2}{1-\lambda(n)^2}\xi_n(1)^2$ are of the form

$$t(0) = 11.9719,\ t(1) = 8.77574,\ t(2) = 2.20528,\ t(3) = 0.0433983,\ t(4) = 0.000125459\ldots$$

and the total value is of the order of 22.9965. As in (60) we get, for the linear form

$$E_+(f) := \int f(x)\epsilon(\exp(|x|))dx, \qquad \forall f \in C_c^\infty(\mathbf{R}) \quad (102)$$

the expression

$$E_+(Q_+f) = -2\epsilon'(1_+)f(0) + \int_0^\infty (f(x)+f(-x))(Q\epsilon)(\exp(x))dx. \quad (103)$$

The equality $Q\epsilon(\rho) = \sum \frac{\lambda(n)^2}{1-\lambda(n)^2} C_n$, together with (100) give a computable expression for $(Q\epsilon)(\rho)$. The graph, after division by $2\epsilon'(1_+)$ and passing to the additive scale, (*i.e.* using $\rho = \exp(x)$) is

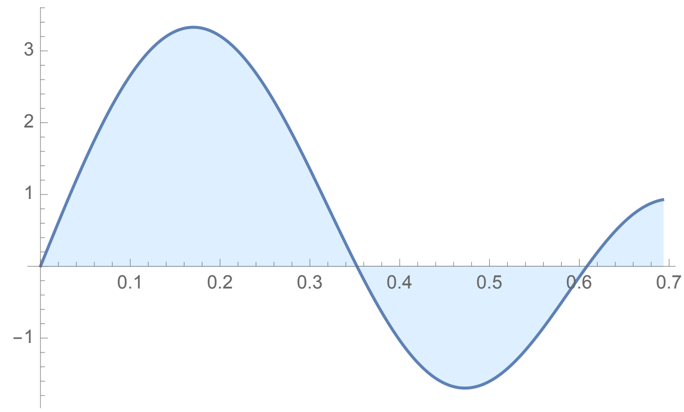

Figure 8. Graph of $(Q\epsilon)(\exp(x))/(2\epsilon'(1_+))$ in $[0, \log 2]$.

In order to determine in which intervals I the form $E_+(Q_+f)$ remains negative, we introduce the associated operator.

Proposition 5.5 *Let $I \subset [-\log 2, \log 2]$ be an interval of length $\leqslant \log 2$.*
(i) The following equality defines a bounded operator $\mathbf{N}_I$ in the Hilbert space $L^2(I, dx)$

$$\langle \eta \mid \mathbf{N}_I(\xi)\rangle = E_+(Q_+f), \quad f = \eta^* * \xi, \quad f(v) = \int \overline{\eta(x)}\xi(x+v)dx. \tag{104}$$

(ii) One has $\mathbf{N}_I = -2\epsilon'(1_+)\,(Id - \mathbf{K}_I)$, where $\mathbf{K}_I$ is the compact operator defined by

$$\langle \eta \mid \mathbf{K}_I(\xi)\rangle = \frac{1}{2\epsilon'(1_+)} \int_{-\log 2}^{\log 2} \int \overline{\eta(x)}\xi(x+v)(Q\epsilon)(\exp(|v|))dxdv. \tag{105}$$

Proof. (i) will follow from (ii), since a compact operator is bounded.
(ii) By applying (103) to $f(v) = \int \overline{\eta(x)}\xi(x+v)dx$ one obtains

$$\langle \eta \mid \mathbf{N}_I(\xi)\rangle = -2\epsilon'(1_+)\langle \eta \mid \xi\rangle + \int_0^\infty (f(x) + f(-x))(Q\epsilon)(\exp(x))dx.$$

Since the length of I is $\leqslant \log 2$, the function $f(v)$ vanishes outside $[-\log 2, \log 2]$ and thus we obtain (105). The proof of the compactness of the operator $\mathbf{K}_I$ is the same as the argument developed at the end of the proof of Theorem 3.6. This shows that $\mathbf{K}_I$ is of Hilbert-Schmidt class. □

Remark 5.6 *The function $Q\epsilon(\rho)$ is 0 for $\rho = 1$. This shows that the integral of diagonal values of the Schwartz kernel defining the compact operator $\mathbf{K}_I$ is 0 independently of the size of I. This result is a clear improvement on the compact operators involved in Theorem 3.6 whose trace is proportional to the length.*

6. Computation of the spectrum of the compact operator $\mathbf{K}_I$

This section is the most elaborate of the paper: it describes the computation of the spectrum of the compact operator $\mathbf{K}_I$ of (105), for an interval $I \subset [-\log 2, \log 2]$ of length $\log 2$. In fact, we shall consider the interval $I = [-\frac{\log 2}{2}, \frac{\log 2}{2}]$. The first difficulty that we encounter concerns formula (98) for the function $Q\epsilon(\rho)$ that involves the prolate spheroidal functions and their derivatives in a complicated way. Fortunately, it is accessible to computer calculations due to the fast decay (72); moreover we show in Appendix F (Lemma F.1) that the sum of the first 11 terms in the series gives a uniform approximation of the function $Q\epsilon(\rho)$ up to 10^{-11}. The second difficulty analyzed in this section has to do with the infinite dimensionality of the Hilbert space on which the operator $\mathbf{K}_I$ acts. This seems, a priori, to preclude the use of computational power to understand its spectrum. Here, the strategy we follow is to use our original idea of "$q \to 1$" that has underlied, since the start, our algebraic work [13, 16, 17]. Thus, we replace the multiplicative group $\mathbf{R}_+^*$ by the discrete subgroup group $q^{\mathbf{Z}}$, and we approximate the infinite dimensional space with a finite dimensional one where the interval I (in additive notation) is replaced by the finite set I_q of size $N \sim \log 2/\log q$, of integral multiples of $\omega = \log q$ which belong to I. It turns out that the natural discretization of the operator $\mathbf{K}_I$ (§6.1) is a Toeplitz matrix and one can investigate its spectrum numerically to see how it varies, when $q \to 1$. What one discovers is that, while for intervals of length a bit smaller than $\log 2$ the largest eigenvalue $\lambda_{\max}$ of $\mathbf{K}_I$ is less than 1, so that $\mathbf{N}_I$ is negative, this no longer holds true when the interval length gets closer to $\log 2$ (see Figure 9). By looking more closely at the spectrum of $\mathbf{K}_I$, one sees that the next to largest eigenvalue stays always smaller than 1! The next step then is to use the powerful theory of self-adjoint Toeplitz matrices [21, 1] showing that the eigenvector ξ associated to the largest eigenvalue fulfills a kind of "baby version" of RH. If one views ξ as a complex-valued function $\xi : I_q \to \mathbf{C}$ by forming the expression

$$\tilde{\xi}(z) = \sum \xi(\log q^j) z^j \in \mathbf{C}[z, z^{-1}],$$

then all the zeros of this function are complex numbers of modulus 1. Their number is $N \sim \log 2/\log q$. By computing these N roots, we noticed that they get distributed as $(N+1)$-th roots of unity except for the trivial root 1. Moreover, one has the symmetry: $z \mapsto z^{-1}$ due to the equality $\tilde{\xi}(z^{-1}) = \tilde{\xi}(z)$. When one rescales the arguments taken in $[-\pi, \pi]$, by multiplication by $(N+1)/2$, their pattern converges when $q \to 1$ (see (110) for the beginning of the patern). The general theory of Toeplitz matrices T also shows [21] that the above roots can be used as a discrete Fourier transform to provide a canonical formula for the lower rank positive Toeplitz matrix $\lambda_{\max}\mathrm{Id} - T$, as a linear combination with positive coefficients $d(j)$ of the form

$$\lambda_{\max}\mathrm{Id} - T = \lambda_{\max} \sum d(j) e(j)$$

where the $e(j)$ are the one dimensional projections (also Toeplitz matrices) associated to the above roots. It turns out that the pattern of the scalar coefficients $d(j)$ also converges when $q \to 1$ (see (113)). The next step is taken in §6.3 and consists of guessing, from the discrete approximation and the above patterns for the roots and the coefficients $d(j)$, a function of the continuous parameter $\rho \in [\frac{1}{2}, 2]$ which approximates $Q\epsilon(\rho)$. This guess is then verified numerically and gives, by a simple estimate, a good approximation of $\mathbf{K}_I$ and a good control of its spectrum using a finite rank operator (see §6.4). Finally, §6.5, 6.6 contain the computation of the spectrum of this finite rank operator as well as the eigenvector of maximal eigenvalue, and the proof that the operator $\mathbf{K}_I$ becomes < 1 in the orthogonal complement of this vector. The proof of the main theorem (Theorem 6.11) is done in §6.7.

6.1 Discrete approximation for variable intervals

We discretize the framework by replacing $\mathbf{R}_+^*$ by $q^{\mathbf{Z}}$, where $q > 1$ and then we let $q \to 1$. By setting $\omega = \log q$ we replace the interval $I = [0, a]$ by its finite intersection with the lattice $\omega\mathbf{Z}$, whose elements $j\omega$ are labeled by $j \in \{0, \ldots, N\}$, where N is the integer part of a/ω. Then we replace integrals by sums and consider, in the finite dimensional Hilbert space $\ell^2(\{0, \ldots, N\})$, the following quadratic form which is the discretized version of (105)

$$\mathcal{Q}_q(\xi) := \omega \sum_{j=0}^{N} \sum_{k=-j}^{N-j} \overline{\xi(j)}\xi(j+k)(Q\epsilon)(q^{|k|}). \tag{106}$$

Following Proposition 5.5, one needs to compare $\mathcal{Q}_q$ with the inner product $2\epsilon'(1_+)\sum_{j=0}^{N} \overline{\xi(j)}\xi(j)$. One expresses (106) as

$$\mathcal{Q}_q(\xi) = \omega\langle \xi \mid \mathcal{T}_q \xi\rangle,$$

where the Toeplitz matrix $\mathcal{T}_q$ is of the form

$$\mathcal{T}_q = \begin{pmatrix} Q\epsilon(1) & Q\epsilon(q) & Q\epsilon(q^2) & Q\epsilon(q^3) & \ldots & Q\epsilon(q^N) \\ Q\epsilon(q) & Q\epsilon(1) & Q\epsilon(q) & Q\epsilon(q^2) & \ldots & Q\epsilon(q^{N-1}) \\ Q\epsilon(q^2) & Q\epsilon(q) & Q\epsilon(1) & Q\epsilon(q) & \ldots & Q\epsilon(q^{N-2}) \\ Q\epsilon(q^3) & Q\epsilon(q^2) & Q\epsilon(q) & Q\epsilon(1) & \ldots & Q\epsilon(q^{N-3}) \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ Q\epsilon(q^N) & Q\epsilon(q^{N-1}) & Q\epsilon(q^{N-2}) & Q\epsilon(q^{N-3}) & \cdots & Q\epsilon(1) \end{pmatrix} \tag{107}$$

Thus we shall compare the largest eigenvalue of $\frac{1}{2\epsilon'(1_+)}\omega\mathcal{T}_q$ with 1 since this tests the positivity of $\mathrm{Id} - \mathbf{K}_I$.

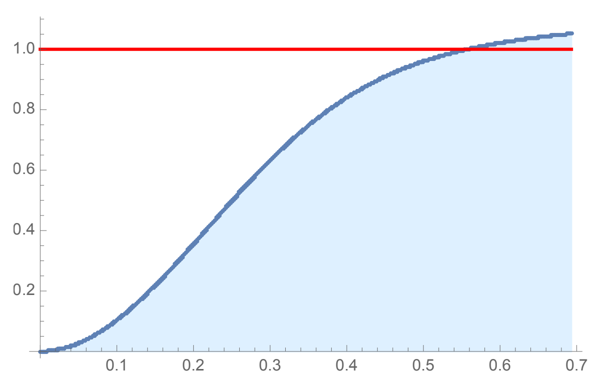

Figure 9. Largest eigenvalue of $\frac{1}{2\epsilon'(1_+)}\omega\mathcal{T}_q$, for $a \in [0, \log 2]$ and $q = \exp(10^{-3})$.

Figure 9 shows that, for $\omega = 10^{-3}$ and $q = \exp(10^{-3})$, the largest eigenvalue of $\frac{1}{2\epsilon'(1_+)}\omega\mathcal{T}_q$, *i.e.* $\lambda \sim 1.05177$, slightly exceeds 1 when one considers the full interval $[0, \log 2]$.

6.2 Discrete approximation and Toeplitz matrices

We now fix the interval $I = [-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$: symmetric and of length $\log 2$. By computing the first eigenvalues of the Toeplitz matrix $\frac{1}{2\epsilon'(1_+)}\omega\mathcal{T}_q$ one finds that the one next to the largest $\lambda = \lambda_1$ is $\lambda_2 \sim 0.687925$: hence well below 1. Thus the lack of positivity of $\mathrm{Id} - \mathbf{K}_I$ is due to a single eigenvector ζ. In the following part we make use of the general theory of Toeplitz matrices [1, 21]. A first key classical result in the theory asserts that the eigenvector for the largest eigenvalue of a self-adjoint Toeplitz matrix is of a very special form since the associated polynomial equation has all its roots of modulus 1. In our notations, this means that if we denote the components of the eigenvector ζ as $\zeta(\log q^j) = \zeta(j\omega)$ which are defined for $|j|\omega \leqslant \frac{1}{2}\log 2$, and let $\tilde{\zeta}(z) = \sum \zeta(j\omega)z^j \in \mathbf{C}[z, z^{-1}]$, then one has the implication

$$z \in \mathbf{C} \ \& \ \tilde{\zeta}(z) = 0 \implies |z| = 1. \tag{108}$$

When we first computed these zeros with the value of q used in §6.1 (*i.e.* $\omega = 10^{-3}$, $q = \exp(10^{-3})$), we found that indeed these zeros are all of modulus 1 and obey the symmetry $z \mapsto \bar{z}$, owing to the fact that the coefficients $\zeta(j\omega)$ are real (they also fulfill $\zeta(-j\omega) = \zeta(j\omega)$). With the symmetric choice of $I = [-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$, the finite number N of elements in $I \cap \omega\mathbf{Z}$ is odd $N = 2m + 1$ and the computation shows that the N roots of $\tilde{\zeta}(z) = 0$ resemble the non-trivial $N + 1$-roots of unity, *i.e.* all of them except $z = 1$. Since they are symmetric these roots are best written in the form

$$z_j^{\pm} = \exp(\pm\frac{2\pi i\alpha_j}{N+1}), \quad j = 1, \dots m, \tag{109}$$

and it turns out that $z = -1$ is also a root and thus it should be added to this list of $2m$ elements. In this way, one discovers that when the roots are labeled as in (109), the obtained numbers α_j, which depend on the choice of $q = \exp(\omega)$, stabilize when $q \to 1$ and the difference $\alpha_j - j$ tends to zero when the index $j \to \infty$. The following is a table showing the first values $\alpha_1, \alpha_2, \dots$, indexed by the integral part *i.e.* $j = \text{IntegerPart}(\alpha_j)$:

$\alpha_1 = 1.33371$	$\alpha_2 = 2.10964$	$\alpha_3 = 3.07018$	$\alpha_4 = 4.0524$	$\alpha_5 = 5.04184$
$\alpha_6 = 6.03484$	$\alpha_7 = 7.02984$	$\alpha_8 = 8.0261$	$\alpha_9 = 9.0232$	$\alpha_{10} = 10.0209$
$\alpha_{11} = 11.019$	$\alpha_{12} = 12.0174$	$\alpha_{13} = 13.016$	$\alpha_{14} = 14.0149$	$\alpha_{15} = 15.0139$
$\alpha_{16} = 16.013$	$\alpha_{17} = 17.0123$	$\alpha_{18} = 18.0116$	$\alpha_{19} = 19.011$	$\alpha_{20} = 20.0104$
$\alpha_{21} = 21.0099$	$\alpha_{22} = 22.0095$	$\alpha_{23} = 23.0091$	$\alpha_{24} = 24.0087$	$\alpha_{25} = 25.0083$
$\alpha_{26} = 26.008$	$\alpha_{27} = 27.0077$	$\alpha_{28} = 28.0074$	$\alpha_{29} = 29.0072$	$\alpha_{30} = 30.007$
$\alpha_{31} = 31.0067$	$\alpha_{32} = 32.0065$	$\alpha_{33} = 33.0063$	$\alpha_{34} = 34.0061$	$\alpha_{35} = 35.006$
$\alpha_{36} = 36.0058$	$\alpha_{37} = 37.0056$	$\alpha_{38} = 38.0055$	$\alpha_{39} = 39.0053$	$\alpha_{40} = 40.0052$
$\alpha_{41} = 41.0051$	$\alpha_{42} = 42.005$	$\alpha_{43} = 43.0048$	$\alpha_{44} = 44.0047$	$\alpha_{45} = 45.0046$
$\alpha_{46} = 46.0045$	$\alpha_{47} = 47.0044$	$\alpha_{48} = 48.0043$	$\alpha_{49} = 49.0043$	$\alpha_{50} = 50.0042$
$\alpha_{51} = 51.0041$	$\alpha_{52} = 52.004$	$\alpha_{53} = 53.0039$	$\alpha_{54} = 54.0039$	$\alpha_{55} = 55.0038$
$\alpha_{56} = 56.0037$	$\alpha_{57} = 57.0037$	$\alpha_{58} = 58.0036$	$\alpha_{59} = 59.0035$	$\alpha_{60} = 60.0035$

(110)

The above list gives some idea of the numerical values of the α_j. The precise numerical values (for $\omega = 1/5000$) are not integers and involve more digits. They can be downloaded at link to download the angles.

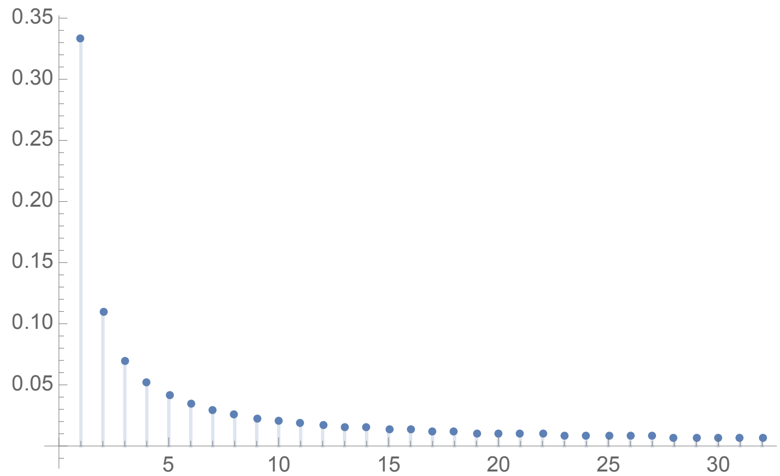

Figure 10. Graph of $\alpha_j - j$.

The second key classical result [1, 21] of the theory of Toeplitz matrices is that for a positive Toeplitz matrix T of co-rank 1 (*i.e.* rank equal to the dimension of the matrix minus one), the face of T in the positive cone is a cone based on a simplex. It follows that there is a unique decomposition of T as a sum of elements of extreme rays of the positive cone. Moreover, the extreme rays of the cone are the rank one (positive) Toeplitz matrices, and they are parametrized (up to a positive multiplicative scalar) by the unit circle $\{z \in \mathbf{C} \mid |z| = 1\}$, formed by rank one projections $e(z)$. Moreover, the unique complex numbers of modulus one involved in the decomposition $T = \sum d(j)e(z_j)$ are precisely the zeros of the polynomial associated to the vector in the kernel of T. We use this result and apply it to the Toeplitz matrix

$$S = \lambda \,\mathrm{Id} - \frac{1}{2\epsilon'(1_+)}\omega \mathcal{T}_q \tag{111}$$

(λ is the largest eigenvalue of $\frac{1}{2\epsilon'(1_+)}\omega \mathcal{T}_q$). By construction and using the simplicity of the largest eigenvalue λ, the obtained Toeplitz matrix S is of co-rank 1 so that it admits a canonical decomposition of the form

$$S = \lambda \sum d(j)e(z_j), \qquad \{z_j\} = \{z \in \mathbf{C} \mid \tilde{\zeta}(z) = 0\}. \tag{112}$$

We computed the list of positive scalars $d(j)$ corresponding to this unique decomposition and found that when $q \to 1$ they behave similarly to the angles, *i.e.* when they are labeled by the corresponding z_j they converge to a fixed value. We give a sample of these values in the next table (113), where we use the same labeling as in (110) so that terms correspond bijectively

$d(1) = 1.17111$	$d(2) = 1.12443$	$d(3) = 1.05904$	$d(4) = 1.03248$	$d(5) = 1.02052$
$d(6) = 1.01414$	$d(7) = 1.01033$	$d(8) = 1.00787$	$d(9) = 1.00619$	$d(10) = 1.005$
$d(11) = 1.00411$	$d(12) = 1.00344$	$d(13) = 1.00292$	$d(14) = 1.00251$	$d(15) = 1.00217$
$d(16) = 1.0019$	$d(17) = 1.00167$	$d(18) = 1.00148$	$d(19) = 1.00132$	$d(20) = 1.00119$
$d(21) = 1.00107$	$d(22) = 1.00097$	$d(23) = 1.00088$	$d(24) = 1.0008$	$d(25) = 1.00073$
$d(26) = 1.00067$	$d(27) = 1.00062$	$d(28) = 1.00057$	$d(29) = 1.00052$	$d(30) = 1.00048$
$d(31) = 1.00045$	$d(32) = 1.00042$	$d(33) = 1.00039$	$d(34) = 1.00036$	$d(35) = 1.00034$
$d(36) = 1.00031$	$d(37) = 1.00029$	$d(38) = 1.00027$	$d(39) = 1.00026$	$d(40) = 1.00024$
$d(41) = 1.00022$	$d(42) = 1.00021$	$d(43) = 1.0002$	$d(44) = 1.00018$	$d(45) = 1.00017$
$d(46) = 1.00016$	$d(47) = 1.00015$	$d(48) = 1.00014$	$d(49) = 1.00013$	$d(50) = 1.00013$
$d(51) = 1.00012$	$d(52) = 1.00011$	$d(53) = 1.0001$	$d(54) = 1.0001$	$d(55) = 1.00009$
$d(56) = 1.00008$	$d(57) = 1.00008$	$d(58) = 1.00007$	$d(59) = 1.00007$	$d(60) = 1.00006$

(113)

Again, this is just to give an idea of these values, and (for $\omega = 1/5000$) the precise numerical values involve more digits and can be downloaded at link to download the coefficients. To achieve a good control of the compact operator $\mathbf{K}_I$ we then need to approximate the function $(Q\epsilon)(\exp(x))$ for all $x \in [0, \log 2]$ and not just on the finite set of multiples of ω. In the next section we shall show how the above Toeplitz decomposition (111) allows one to guess an efficient approximation of the function $(Q\epsilon)(\exp(x))$ by a finite trigonometric sum. This approximation is then shown, by a computer calculation, to give the required control.

6.3 The basic approximation of $(Q\epsilon)(\exp(x))$

By combining (111) and (112), the Toeplitz matrix $T_q = \frac{1}{2\epsilon'(1_+)}\omega\mathcal{T}_q$ can be re-written in the form

$$T_q = \lambda \left(\mathrm{Id} - \sum d(j)e(z_j)\right) \tag{114}$$

where the $e(z_j)$ are the one dimensional Toeplitz projections matrices obtained by conjugating the one dimensional projection on the constant function by the unitary operators

$$(U(\alpha)\xi)(x) := \exp(i2\pi\alpha x/\log 2)\xi(x).$$

This suggests that one can approximate the function $\chi(x) := (Q\epsilon)(\exp(x))/(2\epsilon'(1_+))$ in $[0, \log 2]$ by a trigonometric expression of the form

$$\tau(\lambda, \alpha, d, m)(x) := \frac{2\lambda}{\log 2}\left(\frac{1}{2} + \sum_{n=1}^{m}\left(\cos\frac{2\pi n x}{\log 2} - d(n)\cos\frac{2\pi\alpha_n x}{\log 2}\right)\right). \tag{115}$$

The following fact holds

Fact 6.1 *The distance in $L^1([0, \log 2], dx)$ of the function $\chi(x) := (Q\epsilon)(\exp(|x|))/(2\epsilon'(1_+))$ to the function $\tau(\lambda, \alpha, d, m)(x)$ of (115) (for $m = 1732$, and with the values of the angles α_j and of the coefficients $d(j)$ fixed above) fulfills*

$$2\int_0^{\log 2} |\tau(\lambda, \alpha, d, m)(x) - \chi(x)|dx \sim 0.00122. \tag{116}$$

Proof. The proof is a computer calculation of the $L^1([0, \log 2], dx)$ norm of the difference of the two functions. The function $\tau(\lambda, \alpha, d, m)(x)$ oscillates (these oscillations are visible in the neighborhood of $\log 2$) but it otherwise approximates very well the function $\chi(x)$ as shown by the computer calculation of the L^1 norm of the difference

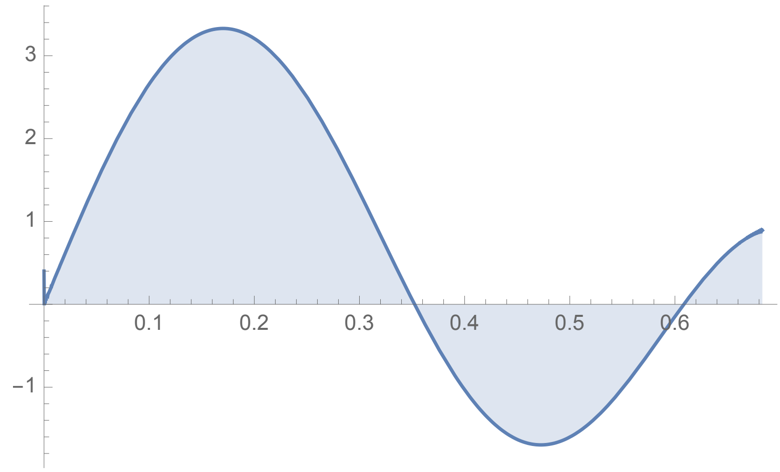

Figure 11. Graph of $\tau(\lambda, \alpha, d, m)(x)$ in $[0, \log 2]$ for $m = 1732$.

To justify (116), one first uses (171) of Appendix F to replace, without any loss, the function $\chi(x) := (Q\epsilon)(\exp(x))/(2\epsilon'(1^+))$ using the contribution of the first 11 terms of the series (170) defining $Q\epsilon$. □

6.4 The approximation of $\mathbf{K}_I$ by a finite rank operator T

Here, the goal is to estimate the quadratic form obtained when one replaces the function $\chi(x)$ by its approximation $\tau(\lambda, \alpha, d, m)(x)$.

Lemma 6.2 *Let $f \in C_c^\infty(\mathbf{R})_{\rm ev}$ be an even smooth function with support contained in the closed interval $[-\log 2, \log 2]$. Then, after rearranging the order of summation, one obtains*

$$\frac{2}{\log 2}\int_{-\log 2}^{\log 2}\left(\frac{1}{2}+\sum_1^\infty \cos\frac{2\pi n x}{\log 2}\right) f(x)dx = f(0) \tag{117}$$

Proof. The equality follows by applying Poisson's formula. Let $L = \mathbf{Z}\log 2$ be the lattice of integral multiples of $\log 2$ and $L^\perp = \mathbf{Z}/\log 2$ be the dual lattice. The Poisson summation formula gives

$$\sum_L f(x) = \frac{1}{\log 2}\sum_{L^\perp}\widehat{f}(y), \qquad \widehat{f}(y) = \int f(u)\exp(-2\pi i u y)du.$$

Since f is even and its support is contained in the closed interval $[-\log 2, \log 2]$ one has,

$$\sum_L f(x) = f(0), \qquad \widehat{f}(y) = \int_{-\log 2}^{\log 2}\exp(2\pi i y x)f(x)dx = \int_{-\log 2}^{\log 2}\cos(2\pi y x)f(x)dx$$

and the Poisson formula thus gives

$$f(0) = \frac{1}{\log 2}\sum_{L^\perp}\widehat{f}(y) = \frac{1}{\log 2}\sum_{\mathbf{Z}}\int_{-\log 2}^{\log 2}\cos\left(\frac{2\pi n x}{\log 2}\right)f(x)dx$$

which gives (117). □

Next, we consider the Hilbert space $\mathcal{H} := L^2([-\frac{1}{2}\log 2, \frac{1}{2}\log 2], dx)$. For $\alpha \in \mathbf{R}$ we let

$$\xi_\alpha(x) := (\log 2)^{-\frac{1}{2}} \exp(\frac{2\pi i \alpha x}{\log 2}), \qquad \forall x \in [-\frac{1}{2}\log 2, \frac{1}{2}\log 2] \tag{118}$$

and $\mathbf{e}_\alpha = |\xi_\alpha\rangle\langle\xi_\alpha|$ be the associated orthogonal projection,

$$\mathbf{e}_\alpha(\xi) = \xi_\alpha\langle\xi_\alpha \mid \xi\rangle, \qquad \forall \xi \in \mathcal{H}.$$

One then has for any $\xi, \eta \in \mathcal{H}$, using the special form (118) of the vector ξ_α

$$\langle\eta \mid \mathbf{e}_\alpha(\xi)\rangle = \langle\eta \mid \xi_\alpha\rangle\langle\xi_\alpha \mid \xi\rangle = \frac{1}{\log 2}\int_{I\times I} \overline{\eta(x)} \exp(\frac{2\pi i\alpha x}{\log 2})\xi(y)\exp(\frac{-2\pi i\alpha y}{\log 2})dxdy$$

so that one obtains

$$\langle\eta \mid \mathbf{e}_\alpha(\xi)\rangle = \frac{1}{\log 2}\int_{-\log 2}^{\log 2}\int \overline{\eta(x)}\xi(x+v)\exp(\frac{-2\pi i\alpha v}{\log 2})dxdv. \tag{119}$$

The following lemma plays a key role in the approximation process

Lemma 6.3 *Let $\tau(\lambda, \alpha, d, m)(x)$ be an approximation of the function $\chi(x)$ so that the L^1 norm of the difference $\tau(\lambda, \alpha, d, m) - \chi$ is $\leqslant \epsilon$. Then the compact operator $\mathbf{K}_I$ of (105), for $I = [-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$, is at a norm distance less than ϵ from the finite rank operator*

$$T = \lambda \sum_{n\in\mathbf{Z}} (\mathbf{e}_n - d(|n|)\mathbf{e}_{\alpha_n}). \tag{120}$$

Here, we set $\alpha_{-n} = -\alpha_n$ $\forall n$ and $d(0) = 0$; while for $n > m$, we set $\alpha_n = n$ and $d(n) = 1$ so that all the terms in the above sum for $|n| > m$ vanish.

Proof. By (115), one has

$$\tau(\lambda, \alpha, d, m)(v) = \frac{\lambda}{\log 2}\sum_{-m}^{m}\left(\exp(\frac{-2\pi i n v}{\log 2}) - d(|n|)\exp(\frac{-2\pi i\alpha_n v}{\log 2})\right)$$

so that, by (119), the operator T of (120) on $\mathcal{H} := L^2([-\frac{1}{2}\log 2, \frac{1}{2}\log 2], dx)$ fulfills the equality

$$\langle\eta \mid T(\xi)\rangle = \int_{-\log 2}^{\log 2}\int \overline{\eta(x)}\xi(x+v)\tau(\lambda, \alpha, d, m)(v)dxdv. \tag{121}$$

The compact operator $\mathbf{K}_I$ of (105) fulfills the same equality, with $\chi(x)$ in place of $\tau(\lambda, \alpha, d, m)(x)$ in the integral. Thus the norm of $\mathbf{K}_I - T$ is bounded by the inequality

$$\left|\int_{-\log 2}^{\log 2}\int \overline{\eta(x)}\xi(x+v)a(v)dxdv\right| \leqslant \|\xi\|\|\eta\|\int_{-\log 2}^{\log 2}|a(v)|dv \tag{122}$$

which follows from the Schwarz inequality $\left|\int \overline{\eta(x)}\xi(x+v)dx\right| \leqslant \|\xi\|\|\eta\|$. □

6.5 The eigenvector of maximal eigenvalue

In order to understand the finite rank operator T of (120) we first construct a vector $\zeta \in \mathcal{H}$ orthogonal to all vectors ξ_{α_n} for $n \neq 0$, using the conventions of Lemma 6.3: *i.e.* for $n > m$ we set $\alpha_n = n$. We first consider the infinite product

$$h(z) := \prod_{n>0}\left(1 - \frac{z^2}{\alpha_n^2}\right)$$

which is convergent likewise the product defining $\frac{\sin(\pi z)}{\pi z}$ and is, by construction, the product of $\frac{\sin(\pi z)}{\pi z}$ by a rational fraction whose role is to replace the zeros $\pm n$ for $n \in \{1, \ldots, m\}$, by the $\pm\alpha_n$. We then consider the Fourier transform of $h(z \log 2)$. We use the notations of Lemma 6.3.

Lemma 6.4 *The Fourier transform $\psi(x) = \frac{1}{\log 2}\widehat{h}(\frac{x}{\log 2})$ of $h(z\log 2)$ has support in the interval $I = [-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$. One has $T\psi = \lambda\psi$ and (using the conventions of Lemma 6.3)*

$$\langle \xi_0 \mid \psi \rangle = (\log 2)^{-\frac{1}{2}}, \qquad \langle \xi_{\alpha_n} \mid \psi \rangle = 0, \qquad \forall n \neq 0. \tag{123}$$

Proof. By construction one has

$$\prod_{0<n\leqslant m} \left(1 - \frac{z^2}{\alpha_n^2}\right) \frac{\sin(\pi z)}{\pi z} = \prod_{0<n\leqslant m} \left(1 - \frac{z^2}{n^2}\right) h(z). \tag{124}$$

The Fourier transform of $\frac{\sin(\pi z)}{\pi z}$ is the characteristic function of the interval $[-\frac{1}{2}, \frac{1}{2}]$, while the Fourier transform of the left hand side of (124) is a distribution with support in the interval $[-\frac{1}{2}, \frac{1}{2}]$. Thus, by (124), the Fourier transform $\widehat{h}$ of the function $h(z)$ fulfills the differential equation of degree $2m$

$$\prod_{0<n\leqslant m} \left(1 + \frac{\partial^2}{(2\pi n)^2}\right) \widehat{h}(x) = 0, \qquad \forall x \notin [-\frac{1}{2}, \frac{1}{2}].$$

Since the space of solutions of this differential equation is made by functions which are linear combinations of the $2m$ trigonometric functions $\exp(\pm 2\pi i n x)$ for $|n| \leqslant m, n \neq 0$, one sees that all these functions are periodic of period 1; thus since $\widehat{h}$ is square integrable it must vanish identically outside $[-\frac{1}{2}, \frac{1}{2}]$. Rescaling by $\log 2$, *i.e.* using $\psi(x) = \frac{1}{\log 2}\widehat{h}(\frac{x}{\log 2})$, one obtains that ψ has support in the interval $I = [-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$. By Fourier inversion, one has for any $n \in \mathbf{Z}$, $n \neq 0$

$$\begin{aligned}\langle \xi_{\alpha_n} \mid \psi \rangle &= (\log 2)^{-\frac{1}{2}} \int_I \psi(x) \exp(-\frac{2\pi i \alpha_n x}{\log 2}) dx = \\ &= (\log 2)^{-\frac{1}{2}} \int \widehat{h}(y) \exp(-2\pi i \alpha_n y) dy = (\log 2)^{-\frac{1}{2}} h(\alpha_n) = 0\end{aligned}$$

which gives (123) (since $h(1) = 1 \Rightarrow \langle \xi_0 \mid \psi \rangle = (\log 2)^{-\frac{1}{2}}$). The orthogonality of ψ to all the vectors ξ_{α_n} shows using (120) that $T\psi = \lambda \sum_{\mathbf{Z}} \mathbf{e}_n \psi = \lambda\psi$, since the vectors ξ_n form an orthonormal basis of $\mathcal{H}$. □

Note that the function ψ is not normalized. The computation of the L^2 norms gives

$$\|\psi\|_2 = (\log 2)^{-\frac{1}{2}} \|h\|_2, \quad \|h\|_2 \sim 1.05143, \quad \text{for } m = 1732 \tag{125}$$

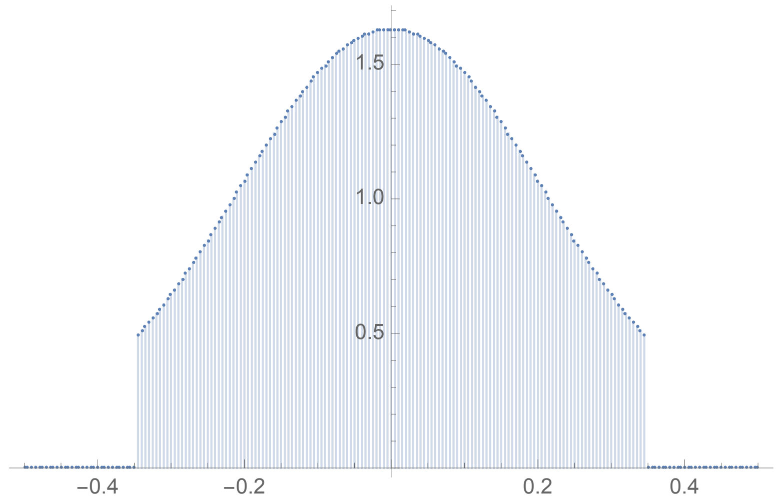

Figure 12. Graph of $\zeta(x) = \psi(x)/\|\psi\|_2$ in $[-\frac{1}{2}, \frac{1}{2}]$.

The important numerical fact is

Fact 6.5 *For $m = 1732$, one has: $\langle \xi_0 \mid \zeta \rangle \sim 0.94865$, where $\zeta(x) = \psi(x)/\|\psi\|_2$.*

6.6 Computation of the spectrum of T

The first method to compute the spectrum of the operator T of (120) is to approximate this finite rank operator using the orthogonal projection $P(n)$ on the linear span of the vectors ξ_j, for $|j| < n$. We use the following expression of the norm square $\|\xi_\alpha - P(n)\xi_\alpha\|^2$.

Lemma 6.6 *Let $(\log \Gamma)^{(2)}$ be the derivative of the logarithmic derivative of the Γ-function, then one has*

$$\|\xi_\alpha - P(n)\xi_\alpha\|^2 = \pi^{-2}\sin^2(\pi\alpha)\left((\log\Gamma)^{(2)}(n-\alpha) + (\log\Gamma)^{(2)}(\alpha+n)\right), \qquad \forall \alpha \in [-n, n] \quad (126)$$

Proof. The components of the vector ξ_α in the basis ξ_m are given as follows

$$(\xi_\alpha)_k = \frac{1}{\log 2}\int_{-\frac{\log(2)}{2}}^{\frac{\log(2)}{2}} \exp\left(\frac{2\pi i(\alpha-k)x}{\log 2}\right) dx = \frac{\sin(\pi(\alpha-k))}{\pi(\alpha-k)}.$$

One then uses the identity, for $a < n$ $\ (\sin^2(\pi(a-n)) = \sin^2(\pi a))$

$$\sum_{k=n}^{\infty}\left(\frac{\sin(\pi(a-k))}{\pi(a-k)}\right)^2 = \frac{\sin^2(\pi(a-n))}{\pi^2}\sum_{k=0}^{\infty}(n-a+k)^{-2} = \pi^{-2}\sin^2(\pi a)(\log\Gamma)^{(2)}(n-a)$$

Similarly for $-n < a$ one has

$$\sum_{k=-\infty}^{-n}\left(\frac{\sin(\pi(a-k))}{\pi(a-k)}\right)^2 = \pi^{-2}\sin^2(\pi a)\sum_{k=-\infty}^{-n}(a-k)^{-2} = \pi^{-2}\sin^2(\pi a)(\log\Gamma)^{(2)}(n+a)$$

which gives (126). □

The equality

$$P(n)\mathbf{e}_\alpha(P(n)\xi) = \langle \xi_\alpha \mid P(n)\xi\rangle P(n)\xi_\alpha = \langle P(n)\xi_\alpha \mid \xi\rangle P(n)\xi_\alpha$$

gives the simple estimate in operator norm

$$\|P(n)\mathbf{e}_\alpha P(n)-\mathbf{e}_\alpha\|\leqslant 2\|\xi_\alpha-P(n)\xi_\alpha\|.$$

This allows one to control the norm of the difference $T-P(m)TP(m)$ as follows

$$\|T-P(m)TP(m)\|\leqslant 2\lambda\sum_{|n|<m}d(|n|)\|\xi_{\alpha_n}-P(m)\xi_{\alpha_n}\|. \tag{127}$$

Using (126) and the asymptotic behavior $(\log\Gamma)^{(2)}(x)=\frac{1}{x}+\frac{1}{2x^2}+O\left(\frac{1}{x}\right)^3$, one obtains a first control of $\|T-P(m)TP(m)\|$. Then, one can compute the eigenvalues of the finite dimensional matrix $P(m)TP(m)$. We did it for $m=1733$, after dividing by λ, to check the highest eigenvalue to be 1. One can then obtain the list of its eigenvalues; the first few, when they are arranged in decreasing order, are the following

$$\{1., 0.652824, 0.027475, 0.000290146, 0.0000877245, 0.0000756436\}.$$

Only the first three stand out as stable positive eigenvalues for T/λ. After multiplication by λ these become

$$\lambda=1.05158,\quad \lambda_2=0.686494,\quad \lambda_3=0.0288921. \tag{128}$$

One can also get the components c_n, on the basis of the ξ_n, of the eigenvector associated to the eigenvalue λ. These components are smaller than 10^{-4} for $n>30$ and their graph near $n=0$ (and for n a bit further) is reproduced here below

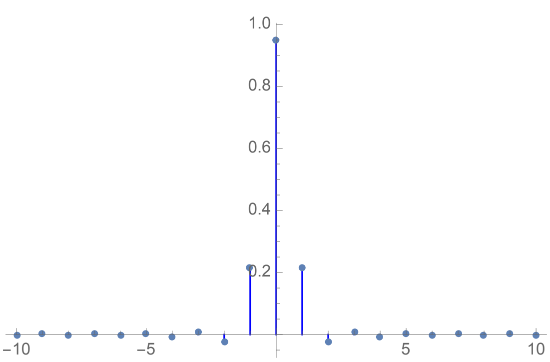

Figure 13. Graph of the components c_n for $|n|<10$.

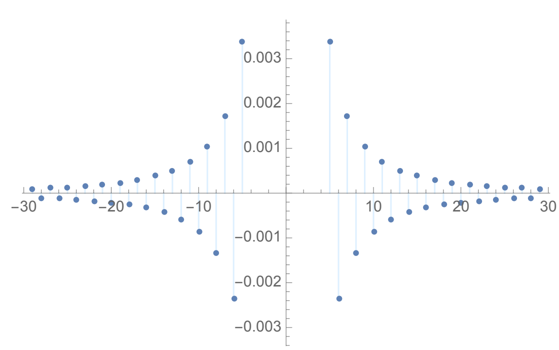

Figure 14. Graph of the components c_n for $7<|n|<30$.

One also checks that the graph (Figure 15) of the reconstructed function $\sum c_n\xi_n$ coincides with the graph (Figure 12) of the theoretical eigenvector of §6.5.

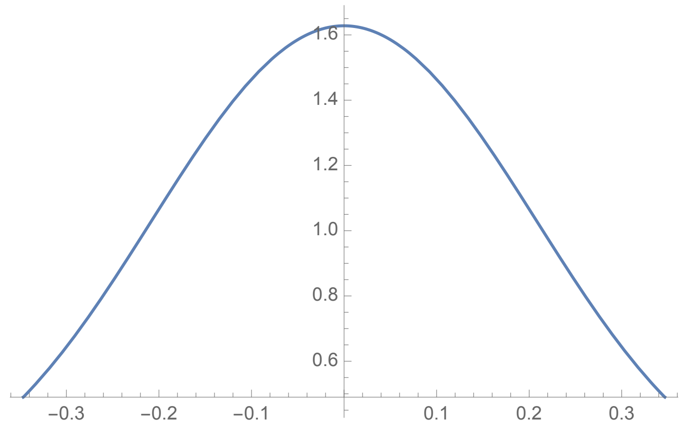

Figure 15. Graph of the reconstructed function $\sum c_n\xi_n$.

The important fact is that the first component $c_0 \sim 0.951067$ is very close to 1.

Remark 6.7 *The components c_n fulfill the symmetry: $c_{-n} = c_n$ for all n. In fact, the finite dimensional real symmetric matrix $M = P(m)TP(m)$ fulfills the further symmetry $M_{-i,-j} = M_{i,j}$ i.e. it commutes with the parity involution. It follows that the eigenvectors associated to simple eigenvalues are even or odd (with respect to the parity involution). One finds, for example, that the eigenvector associated to the second eigenvalue λ_2 is odd, i.e. its components c'_n fulfill $c'_{-n} = -c'_n$ for all n.*

For our purposes, the estimate (127) does not ensure enough precision in the spectrum of T and moreover the need to input the sum (120) gives lengthy computations. We now describe a second method to compute the spectrum of T which improves the precision.

We consider a new basis (ζ_n) of $\mathcal{H} = L^2([-\frac{1}{2}\log 2, \frac{1}{2}\log 2], dx)$ which is no longer orthonormal. More precisely let, with the notation (118),

$$\zeta_0 = \zeta, \qquad \zeta_k = \begin{cases} \xi_k, & \text{for } \ |k| > m, \\ \xi_{-\alpha_{|k|}} & \text{for } \ -m \leqslant k \leqslant -1, \\ \xi_{\alpha_k} & \text{for } \ 1 \leqslant k \leqslant m. \end{cases}$$

One needs to check that the ζ_k, for $|k| \leqslant m$, are linearly independent and this suffices to show that the (ζ_n) form a basis. In fact, by Lemma 6.4, $\zeta_0 = \zeta$ is orthogonal to all ζ_j for $j \neq 0$. In this basis the inner product in $\mathcal{H}$ is given by the matrix J: $J_{i,j} := \langle \zeta_i \mid \zeta_j \rangle$. The operator

$$G := \sum_{n\in\mathbf{Z}} d(|n|)\mathbf{e}_{\alpha_n} \tag{129}$$

is such that

$$\langle \zeta_i \mid G\zeta_j \rangle = \sum_{n\in\mathbf{Z}} d(|n|)\langle \zeta_i \mid \mathbf{e}_{\alpha_n}\zeta_j \rangle = \sum_{n\in\mathbf{Z}} d(|n|)\langle \zeta_i \mid \xi_{\alpha_n}\rangle\langle \xi_{\alpha_n} \mid \zeta_j \rangle = \sum_{n\in\mathbf{Z}} d(|n|)\langle \zeta_i \mid \zeta_n\rangle\langle \zeta_n \mid \zeta_j \rangle.$$

Lemma 6.8 *(i) The spectrum of the operator T of (120) is $\{\lambda_{\max}(1-\beta_j)\}$, where β_j are the eigenvalues of the matrix A: $A_{n,k} := d(|k|)\langle \zeta_n \mid \zeta_k \rangle$.*
(ii) Let $N > m$. The eigenvalues of the matrix A are approximated by the eigenvalues of the

matrix $A^{(N)}$ *defined by:* $A^{(N)}_{i,j} = A_{i,j}$ *if* $|i| \leqslant N$, $|j| \leqslant N$ *and* $A^{(N)}_{i,j} = \delta_{i,j}$ *otherwise, up to an error of* $11\,\epsilon(N)$ *where*

$$\epsilon(N) = \max(e(N), e'(N)), \qquad e(N)^2 = \sum_{|j|\leqslant N} \epsilon(j,N), \quad e'(N)^2 = \sum_{|j|\leqslant N} d(|j|)^2 \epsilon(j,N)$$

with $\epsilon(j,N) := \pi^{-2}\sin^2(\pi\alpha_j)\big((\log\Gamma)^{(2)}(N-\alpha_j) + (\log\Gamma)^{(2)}(\alpha_j+N)\big)$.
(iii) The spectrum of T *is contained in* $\{\lambda_{\max}\} \cup [-2,\lambda_2]$, *where* $\lambda_2 \leqslant 0.772216$.

Proof. By (120): $T = \lambda_{\max}(\mathrm{Id} - \sum_{n\in\mathbf{Z}} d(|n|)\mathbf{e}_{\alpha_n}) = \lambda_{\max}(\mathrm{Id} - G)$, where G is given in (129).

Let $V : \ell^2(\mathbf{Z}) \to \mathcal{H}$ be the linear map: $V(\delta_n) = \zeta_n$ $\forall n \in \mathbf{Z}$, where δ_n is the canonical basis. One has by definition of the matrix J ($J_{i,j} := \langle \zeta_i \mid \zeta_j\rangle$), that

$$\langle V\eta \mid V\eta'\rangle = \langle \eta \mid J\eta'\rangle = \langle J^{\frac12}\eta \mid J^{\frac12}\eta'\rangle.$$

This shows that $U := VJ^{-\frac12} : \ell^2(\mathbf{Z}) \to \mathcal{H}$ is a unitary operator. The spectrum of G ((129)) as an operator in $\mathcal{H}$ is the same as the spectrum of the matrix $U^*GU = J^{-\frac12}LJ^{-\frac12}$, where $L = V^*GV$ thus

$$L_{i,j} = \langle \delta_i \mid V^*GV\delta_j\rangle = \langle \zeta_i \mid G\zeta_j\rangle = \sum_{n\in\mathbf{Z}} d(|n|)\langle \zeta_i \mid \zeta_n\rangle\langle \zeta_n \mid \zeta_j\rangle.$$

The spectrum of G is thus the same as that of the conjugate matrix LJ^{-1}. One has

$$(LJ^{-1})_{i,k} = \sum_{n,j\in\mathbf{Z}} d(|n|)\langle \zeta_i \mid \zeta_n\rangle\langle \zeta_n \mid \zeta_j\rangle (J^{-1})_{j,k} = \sum_{n\in\mathbf{Z}} d(|n|)\langle \zeta_i \mid \zeta_n\rangle \delta_{n,k},$$

since for any $n \in \mathbf{Z}$ one has: $\sum\langle \zeta_n \mid \zeta_j\rangle (J^{-1})_{j,k} = (J\,J^{-1})_{n,k} = \delta_{n,k}$. Thus $(LJ^{-1})_{i,k} = d(|k|)\langle \zeta_i \mid \zeta_k\rangle$ and this proves (i).
(ii) For $|n| > m$ and $|k| > m$, one has: $d(|k|) = 1$, $\zeta_n = \xi_n$, $\zeta_k = \xi_k$, so $A_{n,k} = d(|k|)\langle \zeta_n \mid \zeta_k\rangle = \delta_{n,k}$. The entries $A_{i,j} - A^{(N)}_{i,j}$ of the matrix $A - A^{(N)}$ are non-zero only in the range[12]

$$(i,j) \in [-N,N] \times [-N,N]^c \cup [-N,N]^c \times [-N,N].$$

Thus the operator norm of $A - A^{(N)}$ is less than the sup of the norms of the two blocks corresponding to $[-N,N] \times [-N,N]^c$ and $[-N,N]^c \times [-N,N]$. In turns, the operator norm of these blocks is majored by their Hilbert-Schmidt norm, whose square is

$$\sum_{|i|\leqslant N, |j|>N} |A_{i,j}|^2 = \sum_{|i|\leqslant N} \|\zeta_i - P(N)\zeta_i\|^2, \qquad \sum_{|i|>N, |j|\leqslant N} |A_{i,j}|^2 = \sum_{|j|\leqslant N} d(|j|)^2 \|\zeta_j - P(N)\zeta_j\|^2.$$

Since we assume $N > m$, one has $\zeta_0 = P(N)\zeta_0$, and by (126), for $j \neq 0, |j| \leqslant N$,

$$\|\zeta_j - P(N)\zeta_j\|^2 = \epsilon(j,N) := \pi^{-2}\sin^2(\pi\alpha_j)\left((\log\Gamma)^{(2)}(N-\alpha_j) + (\log\Gamma)^{(2)}(\alpha_j+N)\right).$$

We thus obtain the following control on the operator norm

$$\|A - A^{(N)}\| \leqslant \max(e(N), e'(N)), \;\; e(N)^2 = \sum_{|j|\leqslant N} \epsilon(j,N), \quad e'(N)^2 = \sum_{|j|\leqslant N} d(|j|)^2\epsilon(j,N). \qquad (130)$$

Let $J^{(N)}$ be the matrix defined by: $J^{(N)}_{i,j} = J_{i,j}$ if $|i| \leqslant N$, $|j| \leqslant N$ and $J^{(N)}_{i,j} = \delta_{i,j}$ otherwise. By the same argument as above one obtains

$$\|J - J^{(N)}\| \leqslant e(N). \qquad (131)$$

[12] $[-N,N]^c$ denotes the complement of $[-N,N]$

The matrices J and $J^{(N)}$ are strictly positive. Let $0 < r < 1 < s$ be such that

$$\operatorname{Spec} J \subset [r, s], \qquad \operatorname{Spec} J^{(N)} \subset [r, s], \qquad \|A\| \leqslant s, \quad \|A^{(N)}\| \leqslant s. \tag{132}$$

We shall provide the numerical values of r, s later. Now we estimate the norm difference of the matrices $\Pi = J^{-\frac{1}{2}} A J^{\frac{1}{2}}$ and $\Pi_N = (J^{(N)})^{-\frac{1}{2}} A^{(N)} (J^{(N)})^{\frac{1}{2}}$ which, as shown below, are both positive. We use the equality for strictly positive operators X, X'

$$X^{-\frac{1}{2}} = \frac{1}{\pi}\int_0^\infty (\lambda + X)^{-1}\lambda^{-\frac{1}{2}} d\lambda, \quad X^{-\frac{1}{2}} - X'^{-\frac{1}{2}} = \frac{1}{\pi}\int_0^\infty (\lambda + X)^{-1}(X' - X)(\lambda + X')^{-1}\lambda^{-\frac{1}{2}} d\lambda$$

This gives for $X, X' \geqslant r > 0$ the estimate: $\|X^{-\frac{1}{2}} - X'^{-\frac{1}{2}}\| \leqslant \frac{1}{2} r^{-\frac{3}{2}} \|X - X'\|$. Similarly

$$X^{\frac{1}{2}} - X'^{\frac{1}{2}} = \frac{1}{\pi}\int_0^\infty (\lambda + X')^{-1}(X - X')(\lambda + X)^{-1}\lambda^{\frac{1}{2}} d\lambda$$

which gives the estimate: $\|X^{\frac{1}{2}} - X'^{\frac{1}{2}}\| \leqslant \frac{1}{2} r^{-\frac{1}{2}} \|X - X'\|$. Then we obtain using (132), (130), (131)

$$\|\Pi - \Pi_N\| \leqslant \|(J^{-\frac{1}{2}} - (J^{(N)})^{-\frac{1}{2}}) A J^{\frac{1}{2}}\| + \|(J^{(N)})^{-\frac{1}{2}}(A - A^{(N)}) J^{\frac{1}{2}}\| + \|(J^{(N)})^{-\frac{1}{2}} A^{(N)} (J^{\frac{1}{2}} - (J^{(N)})^{\frac{1}{2}})\|$$

so that

$$\|\Pi - \Pi_N\| \leqslant \frac{1}{2}(s/r)^{\frac{3}{2}} e(N) + (s/r)^{\frac{1}{2}} \max(e(N), e'(N)) + \frac{1}{2}(s/r) e(N) := \epsilon_1(N). \tag{133}$$

The operator $\mathrm{Id} - \Pi$ is compact and self-adjoint, since it corresponds to the matrix $U^*GU = J^{-\frac{1}{2}} L J^{-\frac{1}{2}}$. The operators $A^{(N)}$, $J^{(N)}$ decompose as direct sums in the decomposition $\ell^2(\mathbf{Z}) = \ell^2([-N, N]) \oplus \ell^2([-N, N]^c)$ and both act as identity in $\ell^2([-N, N]^c)$. Their actions in $\ell^2([-N, N])$ are given respectively by the matrices $d(|j|)\langle \zeta_i \mid \zeta_j\rangle$ and $\langle \zeta_i \mid \zeta_j\rangle$. Thus one derives that the operator $J^{(N)}$ is positive and that, as above,

$$\sum_{n,j \in [-N,N]} d(|n|)\langle \zeta_i \mid \zeta_n\rangle\langle \zeta_n \mid \zeta_j\rangle ((J^{(N)})^{-1})_{j,k} = \sum_{n \in [-N,N]} d(|n|)\langle \zeta_i \mid \zeta_n\rangle \delta_{n,k},$$

which shows that both $A^{(N)} J^{(N)}$ and $\Pi_N = (J^{(N)})^{-\frac{1}{2}} A^{(N)} (J^{(N)})^{\frac{1}{2}}$ are positive operators. Thus the operator $\mathrm{Id} - \Pi^{(N)}$ is compact and self-adjoint. Moreover, the norm of the difference $\Pi - \Pi_N$ is majored by $\epsilon_1(N)$. It follows (see [27] Theorem 1.7) that the eigenvalues $\lambda_j, \lambda_j^{(N)}$ of $\mathrm{Id} - \Pi$ and $\mathrm{Id} - \Pi^{(N)}$ arranged in decreasing order, fulfill the inequality: $|\lambda_j - \lambda_j^{(N)}| \leqslant \epsilon_1(N)$, $\forall j$. But these eigenvalues are the same as those of the conjugate operators $\mathrm{Id} - A$ and $\mathrm{Id} - A^{(N)}$. It remains to determine $0 < r < 1 < s$ such that (132) holds. Note first that if $0 < r < 1 < s$ are chosen so that

$$\operatorname{Spec} J \subset [r, s], \qquad \|A\| \leqslant s, \tag{134}$$

then (132) holds since $J^{(N)} = P(N) J P(N) + (1 - P(N))$; so $r \leqslant J \leqslant s$ implies $r \leqslant J^{(N)} \leqslant s$. Also one has: $A^{(N)} = P(N) A P(N) + (1 - P(N))$, so that $\|A^{(N)}\| \leqslant \|A\|$. One then takes $N = 2000$ and uses (130) and (131). Note that the matrix $A^{(N)}$ is not self-adjoint and to bound its norm one uses its decomposition as a sum of a symmetric and an antisymmetric matrix, together with the computation of the eigenvalues of both, which gives the upper bounds 1.533 and 0.0285 for their norms. The value of $\max(e(N), e'(N))$ for $N = 2000$ is ~ 0.017 which provides the bound $s = 1.578$. One finds that the eigenvalues of $J^{(N)}$, for $N = 2000$, are inside the interval $[0.313, 1.346]$ and using $e(N) \sim 0.0145$ one gets $r = 0.299$. This gives $s/r \sim 5.27$ and, by (133), $\epsilon_1(N) \leqslant 11\,\epsilon(N)$: the required bound.

(iii) We use *(ii)* and take $N = 10000$. One gets $\epsilon(N) \sim 0.00740487$, while the first non-zero

eigenvalue of the matrix $A^{(N)}$ is $\beta_2^{(N)} = 0.347112$. Thus by (ii) the first non-zero eigenvalue of the matrix A is $\beta_2 \geqslant \beta_2^{(N)} - 11\epsilon(N) \sim 0.265658$. This shows that the second eigenvalue $\lambda_2 = \lambda_{\max}(1-\beta_2)$ of T fulfills $\lambda_2 \leqslant 0.772216$. ☐

6.7 Proof of Theorem 1

The above computation of the spectrum of the compact operator T together with Lemma 6.3 and the estimate (116) provide the needed information on the spectrum of the compact operator $\mathbf{K}_I$, since both T and $\mathbf{K}_I$ are self-adjoint. Then, by [27] Theorem 1.7, with their eigenvalues arranged in decreasing order and for $\epsilon_1 \simeq 0.00122$, one has:

$$\|\mathbf{K}_I - T\| \leqslant \epsilon_1, \qquad |\lambda_n(\mathbf{K}_I) - \lambda_n(T)| \leqslant \epsilon_1. \tag{135}$$

These bounds allow one to transfer the results of §6.6 from T, to $\mathbf{K}_I$. Up to some computational imprecision which we evaluate later, the results on T are as follows

(i) The three largest eigenvalues of T are given by (128) *i.e.*

$$\lambda_{\max} = 1.05158, \quad \lambda_2 = 0.686494, \quad \lambda_3 = 0.0288921.$$

(ii) The inner product of ζ with the constant function[13] ξ_0 is ~ 0.94865.

Let P_ζ be the orthogonal projection onto $\zeta^\perp := \{\eta \in \mathcal{H} \mid \langle \zeta \mid \eta\rangle = 0\}$. The spectral decomposition

$$T = \lambda_{\max}|\zeta\rangle\langle\zeta| + R, \qquad R \leqslant \lambda_2\, P_\zeta \tag{136}$$

shows that the quadratic form associated to $\mathrm{Id} - T$ is given, using $\mathrm{Id} = |\zeta\rangle\langle\zeta| + P_\zeta$, by

$$\langle \xi \mid (\mathrm{Id} - T)\xi\rangle = (1-\lambda_{\max})|\langle \zeta \mid \xi\rangle|^2 + \langle P_\zeta \xi \mid (P_\zeta - R)\xi\rangle \tag{137}$$

and since $R \leqslant \lambda_2\, P_\zeta$, the last term fulfills

$$\langle P_\zeta \xi \mid (P_\zeta - R)\xi\rangle \geqslant (1-\lambda_2)\|P_\zeta \xi\|^2. \tag{138}$$

Next lemma shows how to restore positivity in a quadratic form which is positive on a codimension one subspace, by adding a rank one quadratic form.

Lemma 6.9 *Let $\mathcal{H}$ be a Hilbert space, $\phi, \psi \in \mathcal{H}$ be unit vectors and P_ϕ the orthogonal projection on $\phi^\perp := \{\eta \in \mathcal{H} \mid \langle \phi \mid \eta\rangle = 0\}$. Let $a, b, c \in \mathbf{R}_+$. Then the following quadratic form on $\mathcal{H}$*

$$B(\xi) := -b|\langle \phi \mid \xi\rangle|^2 + a|\langle \psi \mid \xi\rangle|^2 + c\|P_\phi(\xi)\|^2$$

is positive if and only if

$$a + c \geqslant b, \qquad b(a+c) \leqslant a(b+c)|\langle \phi \mid \psi\rangle|^2. \tag{139}$$

When (139) *holds one has: $B(\xi) \geqslant \epsilon\|\xi\|^2$ $\forall \xi \in \mathcal{H}$, where*

$$2\epsilon = a - b + c - \left((a+b+c)^2 - 4a(b+c)|\langle \phi \mid \psi\rangle|^2\right)^{\frac{1}{2}}. \tag{140}$$

Proof. For any $\xi \in \mathcal{H}$ one has the orthogonal decomposition

$$\xi = P_\phi(\xi) + \phi\langle \phi \mid \xi\rangle = P_\phi(\xi) + e_\phi(\xi).$$

Let $\psi_1 = e_\phi(\psi)$ and $\psi_2 = P_\phi(\psi)$. We can assume $\psi_2 \neq 0$ since otherwise B is positive iff $a \geqslant b$. We can also assume that the scalar product $\alpha = \langle \phi \mid \psi\rangle$ is real. Let then $E \subset \mathcal{H}$ be the two

[13] normalized to be of norm 1

dimensional space generated by ϕ and ψ. Since by hypothesis $c \geqslant 0$, it follows that B is positive iff its restriction to E is positive. In the orthonormal basis of E given by $(\phi, \psi_2/\|\psi_2\|)$ the matrix which represents B is

$$\begin{pmatrix} a\alpha^2 - b & a\alpha\beta \\ a\alpha\beta & a\beta^2 + c \end{pmatrix}, \qquad \alpha = \langle \phi \mid \psi \rangle, \quad \beta = \|\psi_2\|.$$

It is real symmetric, hence its eigenvalues are real: they are both positive iff the trace and the determinant are positive. One also has: $\alpha^2 + \beta^2 = \|\psi\|^2 = 1$. Thus the trace is $a + c - b$. The determinant is: $ca\alpha^2 - ba\beta^2 - bc = a\alpha^2(b + c) - b(a + c)$. The inequality $B(\xi) \geqslant \epsilon\|\xi\|^2$ $\forall \xi \in \mathcal{H}$ then follows from the formula for the eigenvalues of the above matrix, with ϵ being the small one, and the inequality $\epsilon \leqslant c$ which follows from

$$(a + b + c)^2 - 4a(b + c)|\langle \phi \mid \psi \rangle|^2 - (-a + b + c)^2 = 4a(b + c)\left(1 - |\langle \phi \mid \psi \rangle|^2\right).$$

Finally, for $\xi = \xi_1 + \xi_2$, $\xi_1 \in E$, $\xi_2 \in E^\perp$ one has $B(\xi) = B(\xi_1) + B(\xi_2) \geqslant \epsilon\|\xi_1\|^2 + c\|\xi_2\|^2$. □

Lemma 6.10 *Let* $\mathbf{N}_I = -2\epsilon'(1_+)\,(Id - \mathbf{K}_I)$ *be the operator in* $\mathcal{H} = L^2(I)$, $I = [-\frac{1}{2}\log 2, \frac{1}{2}\log 2]$ *which represents the quadratic form associated to* $E_+ \circ Q_+$ *as in Proposition 5.5. Then, with* $\gamma \sim 2.94355$*,*

$$\langle \xi \mid \mathbf{N}_I(\xi) \rangle \leqslant \gamma |\langle \xi_0 \mid \xi \rangle|^2, \quad \forall \xi \in \mathcal{H}. \tag{141}$$

Proof. We first work with T and apply Lemma 6.9, with $\phi = \zeta$, $\psi = \xi_0$. We determine the scalar $a > 0$ to fulfill (139) for $b = \lambda_{\max} - 1$, $c = 1 - \lambda_2$ and the inner product of the two vectors given by $\langle \zeta \mid \xi_0 \rangle$. Since for the above numerical values one has $c > b$, the condition $a + c \geqslant b$ is automatic. The second condition of (139) is

$$a\left((c + b)|\langle \zeta \mid \xi_0 \rangle|^2 - b\right) \geqslant bc.$$

For the above numerical values one has $b \sim 0.05158$, $\langle \zeta \mid \xi_0 \rangle \sim 0.94865$. By Lemma 6.8 one has $c > 0.227784$, then using (140), the following inequality becomes valid, for $a \sim 0.064$, $\epsilon_2 \sim 0.00441$

$$\langle \xi \mid (\mathrm{Id} - T)\xi \rangle + a|\langle \xi_0 \mid \xi \rangle|^2 \geqslant \epsilon_2\|\xi\|^2, \qquad \forall \xi \in \mathcal{H}.$$

By (135), one has $\|\mathbf{K}_I - T\| \leqslant \epsilon_1$, where $\epsilon_1 \simeq 0.00122 < \epsilon_2$, thus

$$\langle \xi \mid (\mathrm{Id} - \mathbf{K}_I)\xi \rangle + a|\langle \xi_0 \mid \xi \rangle|^2 \geqslant (\epsilon_2 - \epsilon_1)\|\xi\|^2, \qquad \forall \xi \in \mathcal{H}$$

which gives (141) after multiplication by $-2\epsilon'(1_+)$. □

We can finally state our main result

Theorem 6.11 *Let* $g \in C_c^\infty(\mathbf{R}_+^*)$ *be a smooth function with support in the interval* $[2^{-1/2}, 2^{1/2}]$ *and whose Fourier transform vanishes at* $-\frac{i}{2}$*. Let* $\mathbf{S}$ *be the orthogonal projection of* $L^2(\mathbf{R})_{\mathrm{ev}}$ *onto the subspace of even functions which vanish as well as their Fourier transform in the interval* $[-1, 1]$*. Then*

$$W_\infty(g * g^*) \geqslant \mathrm{Tr}(\vartheta(g)\,\mathbf{S}\,\vartheta(g)^*) - c\,|\widehat{g}(0)|^2, \qquad c = \frac{4\gamma}{\log 2}. \tag{142}$$

Proof. By Theorem 4.6 one has, for $f = g * g^*$,

$$\mathrm{Tr}(\vartheta(f)\mathbf{S}) = W_\infty(f) + \int f(\rho^{-1})\epsilon(\rho)d^*\rho = W_\infty(f) + E(f). \tag{143}$$

Let $k(u) := u^{\frac{1}{2}} \int_0^u v^{-\frac{1}{2}} g(v)\, d^*v$. One has: $0 = \widehat{g}(-\frac{i}{2}) = \int_0^\infty v^{-\frac{1}{2}} g(v)\, d^*v$, thus the support of k is contained in $[2^{-1/2}, 2^{1/2}]$. Moreover: $k = Y * g$, $k^* = Y^* * g^*$, $k * k^* = Y^* * Y * f$ where, as in

Lemma 3.3, $Y(\rho)=0$ for $\rho<1$, $Y(\rho)=\rho^{\frac12}$ for $\rho\geqslant 1$ and $Y^*(\rho)=Y(\rho^{-1})$. Thus one gets

$$Q(k*k^*)=g*g^*=f, \qquad \widehat{k}(0)=-2\,\widehat{g}(0) \tag{144}$$

where the second equality follows using integration by parts from

$$\widehat{k}(0)=\int_0^\infty k(u)d^*u=\int_0^\infty\left(\int_0^u v^{-\frac32}g(v)\,dv\right)u^{-\frac12}du=-\int_0^\infty u^{-\frac32}g(u)2u^{\frac12}du=-2\,\widehat{g}(0).$$

One thus obtains

$$\int f(\rho^{-1})\epsilon(\rho)d^*\rho=E\circ Q(k*k^*).$$

Let $\xi(x):=k(\exp(x))$. One has: $\xi\in\mathcal{H}=L^2([-\frac12\log 2,\frac12\log 2])$ and using (104) of Proposition 5.5

$$E\circ Q(k*k^*)=E_+(Q_+(\xi*\xi^*))=\langle\xi\mid\mathbf{N}_I(\xi)\rangle.$$

Then, by Lemma 6.10 one gets, using $\langle\xi_0\mid\xi\rangle=(\log 2)^{-1/2}\widehat{\xi}(0)=(\log 2)^{-1/2}\widehat{k}(0)$

$$E(f)=E\circ Q(k*k^*)=\langle\xi\mid\mathbf{N}_I(\xi)\rangle\leqslant\gamma|\langle\xi_0\mid\xi\rangle|^2=\frac{\gamma}{\log 2}|\widehat{k}(0)|^2=\frac{4\gamma}{\log 2}|\widehat{g}(0)|^2,$$

which gives the required inequality. ☐

Remark 6.12 *By* (135)*, the first eigenvalue* $\lambda_1(\mathbf{K}_I)$ *of* $\mathbf{K}_I$ *fulfills* $|\lambda_1(\mathbf{K}_I)-\lambda_{\max}|\leqslant\epsilon_1$ *while* $\lambda_{\max}=1.05158$ *and* $\epsilon_1\simeq 0.00122$*. Thus, since* $C_c^\infty((-\frac12\log 2,\frac12\log 2))$ *is dense in the Hilbert space* $\mathcal{H}=L^2([-\frac12\log 2,\frac12\log 2])$*, there exists a unit vector* $\xi\in C_c^\infty((-\frac12\log 2,\frac12\log 2))$ *such that* $\mathbf{K}_I(\xi)\sim\lambda_1(\mathbf{K}_I)\xi$*. It follows, using* $\mathbf{N}_I=-2\epsilon'(1_+)\,(Id-\mathbf{K}_I)$*, that*

$$\langle\xi\mid\mathbf{N}_I(\xi)\rangle\geqslant 2\epsilon'(1_+)(1.05-1)\|\xi\|^2\geqslant 0.1\,\epsilon'(1_+)|\langle\xi_0\mid\xi\rangle|^2$$

Let then $h(\rho):=\xi(\log\rho)$ *and* $g(\rho):=(\frac12-\rho\partial_\rho)h(\rho)$*, so that* $g(\rho)=\eta(\log\rho)$ *for* $\eta=\frac12\xi-\xi'$*. One has* $\widehat{g}(-\frac{i}{2})=0$ *and as in the proof of Theorem 6.11 one obtains*

$$E(g*g^*)=E\circ Q(h*h^*)=\langle\xi\mid\mathbf{N}_I(\xi)\rangle\geqslant 0.1\,\epsilon'(1_+)|\langle\xi_0\mid\xi\rangle|^2>13|\widehat{g}(0)|^2.$$

Thus by (143) *one gets*

$$W_\infty(g*g^*)=\mathrm{Tr}(\vartheta(g)\,\mathbf{S}\,\vartheta(g)^*)-E(g*g^*)<\mathrm{Tr}(\vartheta(g)\,\mathbf{S}\,\vartheta(g)^*)-13|\widehat{g}(0)|^2.$$

This shows that the best constant c fulfilling (142) *is such that* $13<c<17$*.*

Appendix A. Fourier versus Mellin transforms

We use the convolution algebra $C_c^\infty(\mathbf{R}_+^*)$ of smooth complex valued functions with compact support on the multiplicative group $\mathbf{R}_+^*$. Its convolution product and involution are given by

$$(f*g)(u):=\int f(v)g(u/v)d^*v, \qquad f^*(u):=\overline{f(u^{-1})}. \tag{145}$$

The (multiplicative) Fourier transform of f (see (22))

$$\hat{f}(s)=\int_0^\infty f(u)u^{-is}d^*u$$

transforms convolution into pointwise product and the involution into the pointwise complex conjugation, $s\in\mathbf{R}$. For complex values of s, the evaluation $f\mapsto\hat{f}(s)$ is still multiplicative but no longer compatible with the involution.

The translation to formulas using the Mellin transform is done in (41) and uses the isomorphism

$$k \stackrel{\sim}{\mapsto} \Delta^{1/2}(k) = f, \qquad f(x) := x^{1/2}k(x) \tag{146}$$

which respects the convolution product, and transforms $x^{-1}k(x^{-1})$ into $f(x^{-1})$. Hence, after taking complex conjugates, the natural involution $k \mapsto \bar{k}^\sharp$ becomes $f \mapsto f^*$. The Mellin transform $\tilde{k}(z) := \int_0^\infty k(u)u^z d^*u$ is related to the (multiplicative) Fourier transform of f by (41) *i.e.*

$$\tilde{k}(\frac{1}{2} + is) = \int_0^\infty k(u)u^{\frac{1}{2}+is}d^*u = \int_0^\infty f(u)u^{is}d^*u = \hat{f}(-s), \tag{147}$$

where the sign in $-s$ is due to the convention for the multiplicative Fourier transform (22).

Appendix B. Explicit formula

In this appendix, we gather different sources on the normalization of the archimedean contribution to the explicit formula. Following [7], one defines the Mellin transform of a function $f \in C_c^\infty(\mathbf{R}_+^*)$ as

$$\tilde{f}(s) := \int_0^\infty f(x)x^{s-1}dx. \tag{148}$$

Then, with $f^\sharp(x) := x^{-1}f(x^{-1})$ the explicit formula takes the form

$$\sum_\rho \tilde{f}(\rho) = \int_0^\infty f(x)dx + \int_0^\infty f^\sharp(x)dx - \sum_v \mathcal{W}_v(f), \tag{149}$$

where v runs over all places $\{\mathbf{R}, 2, 3, 5, \ldots\}$ of $\mathbf{Q}$, the sum on the left hand side is over all complex zeros ρ of the Riemann zeta function, and for $v = p$

$$\mathcal{W}_p(f) = (\log p) \sum_{m=1}^\infty \left(f(p^m) + f^\sharp(p^m)\right). \tag{150}$$

The archimedean distribution is defined as

$$\mathcal{W}_\mathbf{R}(f) := (\log 4\pi + \gamma)f(1) + \int_1^\infty \left(f(x) + f^\sharp(x) - \frac{2}{x}f(1)\right)\frac{dx}{x - x^{-1}}. \tag{151}$$

One then has

$$\mathcal{W}_\mathbf{R}(f) = (\log \pi)f(1) - \frac{1}{2\pi i}\int_{1/2+iw} \Re\left(\frac{\Gamma'}{\Gamma}\left(\frac{w}{2}\right)\right)\tilde{f}(w)dw. \tag{152}$$

In [6] and [8] a positivity result for the distribution $\mathcal{W}_\infty = -\mathcal{W}_\mathbf{R}$ is proven, (for test functions with support in a small enough interval around 1), by writing the distribution $\mathcal{W}_\infty$ in terms of the Mellin transform of the test function as follows

$$\mathcal{W}_\infty(f) = \int_{w=1/2+i\tau} h_+(\tau)\tilde{f}(w)\frac{d\tau}{2\pi}. \tag{153}$$

The function $h_+(\tau)$ is

$$h_+(\tau) = -\log \pi + \Re(\lambda(1/4 + i\tau/2)), \qquad \lambda(z) = \Gamma'(z)/\Gamma(z). \tag{154}$$

It is the derivative of $2\,\theta(\tau)$, where θ is the Riemann-Siegel angular function defined as

$$\theta(E) = -\frac{E}{2}\log \pi + \Im \log \Gamma\left(\frac{1}{4} + i\frac{E}{2}\right), \tag{155}$$

with $\log\Gamma(s)$, for $\Re(s) > 0$, the branch of the log which is real for s real.
In order to reflect the unitarity of the scaling action it is convenient to use the automorphism of $C_c^\infty(\mathbf{R}_+^*)$, $f \mapsto \Delta^{1/2} f$, $\Delta^{1/2} f(x) := x^{1/2} f(x)$ which replaces the involution $f \mapsto \overline{f}^\sharp$ by the involution $f \mapsto f^*$ of the convolution C^*-algebra and the restriction of the Mellin transform to the critical line by the Fourier transform. One has, for any place v, $W_v(f) := \mathcal{W}_v(\Delta^{-1/2} f)$, $\forall f \in C_c^\infty(\mathbf{R}_+^*)$.

Appendix C. Positivity criterion

This appendix shows that one may impose finitely many vanishing conditions to test functions without altering the validity of Weil's positivity criterion. We follow [36] and state the following equivalence, using the Mellin transform

Proposition C.1 *Let $Z \subset \mathbf{C}$ be the set of non-trivial zeros of the Riemann zeta function and $F \subset \mathbf{C}$ a finite set disjoint from Z and containing $\{0,1\}$, then*

$$RH \iff \sum_v \mathcal{W}_v(g * \bar{g}^\sharp) \leqslant 0, \quad \forall g \in C_c^\infty(\mathbf{R}_+^*) \mid \tilde{g}(z) = 0, \ \forall z \in F. \tag{156}$$

Proof. The implication "⇒" follows from the explicit formula (149) and the hypothesis $\{0,1\} \subset F$. Conversely, the proof of Proposition 1 of [36] applies verbatim, provided one first refines the proof of Lemma 1 of *op.cit.* by showing that, given $\epsilon > 0$ and $\rho_0 \in Z$, there exists $g_0 \in C_c^\infty(\mathbf{R}_+^*)$ such that

$$\tilde{g}_0(z) = 0, \quad \forall z \in F; \quad \tilde{g}_0(\rho_0) = 1; \quad |\tilde{g}_0(\rho)| \leqslant \epsilon/|\rho - \rho_0|^2, \quad \forall \rho \in Z, \ \rho \neq \rho_0.$$

In order to fulfill the additional vanishing condition: $\tilde{g}_0(z) = 0, \forall z \in F$, one adjoins F to the finite set of zeros fulfilling $|\rho - \rho_0| < R$ (same notation as in Proposition 1 of [36]), and one then proceeds exactly as in *op.cit.* ☐

Appendix D. Quantized calculus redux

Let C be a locally compact abelian group endowed with the proper homomorphism

$$\mathrm{Mod} : C \to \mathbf{R}_+^*, \qquad \mathrm{Mod}(u) = |u| \quad u \in C.$$

We let $\widehat{C}$ be the Pontrjagin dual of C endowed with its Haar measure. The elements $f \in L^\infty(\widehat{C})$ act as multiplication operators on the Hilbert space $\mathcal{H} := L^2(\widehat{C})$. We define the "quantized" differential of f to be the operator

$$đf := [H, f] = Hf - fH, \tag{157}$$

where the operator H on $\mathcal{H}$ is

$$H := 2\mathbf{F}_C \, \mathbf{1}_P \, \mathbf{F}_C^{-1} - 1, \tag{158}$$

where $\mathbf{F}_C : L^2(C) \to \mathcal{H}$ is the Fourier transform, and $\mathbf{1}_P$ is the multiplication by the characteristic function of the set $P = \{u \in C \mid |u| \geqslant 1\}$.

We take the case $C = \mathbf{R}$ with module $\exp : \mathbf{R} \to \mathbf{R}_+^*$ considered in this paper and identify the dual $\widehat{C} \sim \mathbf{R}$ using the bi-character $\nu(s,t) := \exp(-ist)$ which corresponds to (21) under the isomorphism given by the module. We give a "geometric" proof of the following Lemma (see [10] Chapter IV for the general theory, a compact operator has infinite order when its characteristic values form a sequence of rapid decay; this implies that it is of trace class).

Lemma D.1 *For $f \in \mathcal{S}(\widehat{C})$ the quantized differential $[H, f]$ is an infinitesimal of infinite order and in particular a trace class operator.*

Proof. Let us work in the Hilbert space $L^2(C)$ so that the action of $K = \mathbf{F}_C^{-1} f \mathbf{F}_C$ is a convolution operator with Schwartz kernel $k(x,y) = \widehat{f}(x-y)$. The projection $\mathbf{1}_P$ is the multiplication by the characteristic function of the halfline $[0,\infty]$. It is enough to show that the operator $PK(1-P)$ is of infinite order. After precomposition with the symmetry $\sigma(\xi)(x) := \xi(-x)$ the Schwartz kernel of $PK(1-P)\sigma$ is $h(x,y) = P(x)\widehat{f}(x+y)P(y)$. Let $\phi \in C^\infty(\mathbf{R})$ be a smooth function which is identically 0 for $x \leqslant -1$ and identically 1 for $x \geqslant 0$. Let $g = \widehat{f}$ and T be the operator in $L^2(\mathbf{R})$ given by

$$T\xi(x) := \int \phi(x) g(x+y) \phi(y) \xi(y) dy.$$

One has $PTP = PK(1-P)\sigma$ and thus it is enough to show that T is of infinite order. Let $A := -\partial_x^2 + x^2$ be the harmonic oscillator, it is enough to show that the operator $A^n T$ is bounded for any $n > 0$. Indeed the eigenvalues of A are the positive integers with multiplicity 1 and the above boundedness ensures that the characteristic values of T are of rapid decay. Now the Schwartz kernel of $A^n T$ is a finite linear combination of products of the form

$$\phi(y)\phi(x)^{(\ell')} x^k g^{(\ell)}(x+y).$$

Since $g = \widehat{f} \in \mathcal{S}(\mathbf{R})$ the derivatives $g^{(\ell)}$ are of rapid decay and for any given $m > 0$ one has an inequality of the form $|g^{(\ell)}(a)| \leqslant C_m (3+a)^{-m}$ for all $a \geqslant -2$. it follows that one controls the Hilbert Schmidt norm by the square root of the integral

$$C_m^2 \int_{-1}^{\infty} \int_{-1}^{\infty} |\phi(y)\phi(x)^{(\ell')}|^2 |x|^{2k} (3+x+y)^{-m} dx dy$$

which is finite for m large enough. This shows as required that $A^n T$ is bounded for any $n > 0$. ☐

Remark D.2 *One can give two alternate proofs of Lemma D.1. The first uses the conformal invariance of the quantized calculus to get a unitary operator $U : L^2(S^1) \to L^2(\mathbf{R})$ of the form $(U\xi)(t) := \frac{\pi^{-1/2}}{t+i}\,\xi(\frac{t-i}{t+i})$ which conjugates, up to sign, the Hilbert transform H (which acts in $L^2(\widehat{C})$) by the operator $2P_{H^2} - 1$ where P_{H^2} is the orthogonal projection on boundary values of holomorphic functions. Moreover the conjugate of the multiplication operator by $f \in \mathcal{S}(\mathbf{R})$ is the multiplication by the smooth function $g(z) = f(i(1+z)/(1-z))$. Then the result follows since the quantized differential of a smooth function $g \in C^\infty(S^1)$ is of the form $2\sum \widehat{g}(n)[P_{H^2}, z^n]$ which is of infinite order because the $\widehat{g}(n)$ are of rapid decay. The fact that $g \in C^\infty(S^1)$ comes from the smoothness os the extension of a Schwartz function to $P^1(\mathbf{R})$ by the value 0 at ∞.*
Another instructive alternate proof is to estimate directly, for $f \in \mathcal{S}(\mathbf{R})$, the Schwartz kernel given by

$$k(x,y) = \frac{f(x) - f(y)}{x - y}.$$

Appendix E. Signs and normalizations

We follow [32] and use the classical formula expressing the Fourier transform as a composition of the inversion

$$I(f)(s) := f(s^{-1}) \tag{159}$$

and a multiplicative convolution operator. In our framework the unitary u is given by the ratio of archimedean local factors on the critical line

$$u(s) = \frac{\pi^{-z/2}\Gamma(z/2)}{\pi^{-(1-z)/2}\Gamma((1-z)/2)}, \qquad z = 1/2 + is. \tag{160}$$

In terms of the Riemann-Siegel angular function (155), one has

$$u(s) = e^{2\,i\,\theta(s)}, \tag{161}$$

so that the function $Z(t) := e^{i\theta(t)}\zeta(\frac{1}{2}+it)$ is real valued. Indeed, this follows from the functional equation since the complete zeta function $\zeta_{\mathbf{Q}}(z) := \pi^{-z/2}\Gamma(z/2)\zeta(z)$ is real valued on the critical line. The quantized differential $đf$ of f is given by the kernel

$$k(s,t) = \frac{i}{\pi}\,\frac{f(s)-f(t)}{s-t}. \tag{162}$$

Thus when one takes the logarithmic derivative of u one obtains on the diagonal

$$u^* đu(s) = e^{-2\,i\,\theta(s)}\frac{i}{\pi}\partial_s e^{2\,i\,\theta(s)} = -\frac{2}{\pi}\partial_s\theta(s) \implies \frac{1}{2}u^* đu(s) = \frac{-2\partial_s\theta(s)}{2\pi}. \tag{163}$$

One can then write

$$\mathrm{Tr}(\hat{h}_1\left(\frac{1}{2}u^{-1}đu\right)\hat{h}_2) = -\int \hat{h}_1(t)\hat{h}_2(t)\frac{2\partial_t\theta(t)}{2\pi}dt. \tag{164}$$

This corresponds to (153) since $\mathcal{W}_{\mathbf{R}} = -\mathcal{W}_\infty$ and to the semi-local trace formula

$$\mathrm{Tr}(\hat{h}_1\left(\frac{1}{2}u^{-1}đu\right)\hat{h}_2) = \sum_{v\in S}\int'_{\mathbf{Q}_v^*}\frac{|w|^{1/2}}{|1-w|}\,h(w)d^*w, \quad h = h_1 * h_2, \tag{165}$$

for the single archimedean place.

Appendix F. Issues of convergence

We gather several inequalities which ensure the convergence of the series (99) of Proposition 5.3. We first consider the terms

$$A_n(\rho) := \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}\;\rho^{1/2}\int_{\rho^{-1}}^1 (D_u\xi_n)(x)(D_u\zeta_n)(\rho x)dx.$$

We estimate the integral using Schwarz's inequality

$$\left|\rho^{1/2}\int_{\rho^{-1}}^1 (D_u\xi_n)(x)(D_u\zeta_n)(\rho x)dx\right| \leqslant \left(\int_{\rho^{-1}}^1 (D_u\xi_n)(x)^2dx\right)^{\frac{1}{2}}\left(\int_{\rho^{-1}}^1 (D_u\zeta_n)(\rho x)^2\rho dx\right)^{\frac{1}{2}}.$$

One has, using $D_u(f)(x) = x\partial_x f(x)$

$$\int_{\rho^{-1}}^1 (D_u\zeta_n)(\rho x)^2\rho dx = \int_1^\rho (D_u\zeta_n)(y)^2dy \leqslant \rho^2\int_1^\rho (\partial_y\zeta_n)(y)^2dy.$$

With $\zeta_n(x) = \frac{1}{\sqrt{1-\lambda(n)^2}}\eta_n(x)$ and $\eta_n = \mathbf{F}_{e_{\mathbf{R}}}\xi_n$ one thus obtains

$$\int_1^\rho (\partial_y\zeta_n)^2(y)dy = \frac{1}{1-\lambda(n)^2}\int_1^\rho (\partial_y\eta_n)^2(y)dy \leqslant \frac{1}{1-\lambda(n)^2}(2\pi)^2,$$

since $\partial_y \eta_n$ is the Fourier transform of $2\pi i x \xi_n(x)$ whose L^2-norm is bounded by 2π. We thus get

$$\left(\int_{\rho^{-1}}^{1} (D_u \zeta_n)^2(\rho x)\rho dx\right)^{\frac{1}{2}} \leqslant \rho \frac{2\pi}{\sqrt{1-\lambda(n)^2}}.$$

To estimate $\int_{\rho^{-1}}^{1} (D_u \xi_n)(x)^2 dx$, we rewrite the equality (67) as follows

$$(\mathbf{W} f)(x) = -\left(1-x^2\right) f''(x) + 2x f'(x) + 4\pi^2 x^2 f(x), \tag{166}$$

so that since ξ_n is an eigenvector of $\mathbf{W}$ (*i.e.* $\mathbf{W}\xi_n = \chi_{2n}^{2\pi}\xi_n$), using the notations of [33], we get

$$D_u(\xi_n)(x) = \frac{1}{2}\left(1-x^2\right)\xi_n''(x) + (\chi_{2n}^{2\pi} - 2\pi^2 x^2)\xi_n(x).$$

Assuming $n \geqslant 3$ to ensure $\chi_{2n}^{2\pi} \geqslant 2\pi^2$ one then derives

$$\|D_u(\xi_n)\| \leqslant \chi_{2n}^{2\pi} + \frac{1}{2}\left(\int_0^1 (\xi_n''(x))^2(1-x^2)^2 dx\right)^{\frac{1}{2}}.$$

By [33] (Theorem 3.6) one has (note the different normalization of inner product due to (16))

$$\left(\int_0^1 (\xi_n''(x))^2(1-x^2)^2 dx\right)^{\frac{1}{2}} \leqslant (2n)^2 + (6\pi+1)2n + 3(2\pi+1)^2, \tag{167}$$

while the eigenvalues $\chi_{2n}^{2\pi}$ fulfill (see *op.cit.*): $\chi_{2n}^{2\pi} \leqslant 2n(2n+1) + (2\pi)^2$. Thus, one obtains the inequality

$$\|D_u(\xi_n)\| \leqslant 8n^2 + (6\pi+2)2n + 16\pi^2 + 12\pi + 1$$

and the following uniform bound (take $\rho \leqslant 2$)

$$|A_n(\rho)| \leqslant \frac{\lambda(n)}{1-\lambda(n)^2} 4\pi(8n^2 + (6\pi+2)2n + 16\pi^2 + 12\pi + 1), \qquad \forall \rho,\ 1 \leqslant \rho \leqslant 2. \tag{168}$$

We then consider the terms

$$B_n(\rho) := \frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}} \left(\rho^{-1/2}(D_u\xi_n)(\rho^{-1})\zeta_n(1) - \rho^{1/2}\xi_n(1)(D_u\zeta_n)(\rho)\right).$$

By (101), one has $|\xi_n(1)| \leqslant \sqrt{2n+\frac{1}{2}}$. One also has $\zeta_n = \frac{1}{\sqrt{1-\lambda(n)^2}}\eta_n$ and $\eta_n = \mathbf{F}_{e_{\mathbf{R}}}\xi_n$ thus

$$(D_u\zeta_n)(\rho) = \frac{1}{\sqrt{1-\lambda(n)^2}}\ \rho\eta_n'(\rho) \implies |(D_u\zeta_n)(\rho)| \leqslant \frac{8\pi}{\sqrt{1-\lambda(n)^2}}, \qquad \forall \rho,\ 1 \leqslant \rho \leqslant 2$$

using the equality $\eta_n'(\rho) = -4\pi \int_0^1 \sin(2\pi\rho x)\xi_n(x) x dx$ and Schwarz's inequality. Hence

$$\frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}\left|\rho^{1/2}\xi_n(1)(D_u\zeta_n)(\rho)\right| \leqslant \frac{\lambda(n)}{1-\lambda(n)^2} 8\pi\sqrt{2(2n+\frac{1}{2})}, \qquad \forall \rho,\ 1 \leqslant \rho \leqslant 2.$$

By (75) one gets: $\eta_n(x) = \lambda(n)\xi_n(x)$, for $x \in [0,1]$ thus one obtains by proportionality

$$(D_u\xi_n)(\rho^{-1})\zeta_n(1) = \frac{1}{\sqrt{1-\lambda(n)^2}}(D_u\xi_n)(\rho^{-1})\eta_n(1) = \frac{1}{\sqrt{1-\lambda(n)^2}}(D_u\eta_n)(\rho^{-1})\xi_n(1)$$

and the above bound for $\eta_n'(y) = -4\pi \int_0^1 \sin(2\pi y x)\xi_n(x) x dx$, applied for $y = \rho^{-1}$ thus gives

$$|(D_u\xi_n)(\rho^{-1})\zeta_n(1)| \leqslant \frac{4\pi}{\sqrt{1-\lambda(n)^2}}\sqrt{2n+\frac{1}{2}}$$

so that

$$\frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}|\rho^{-1/2}(D_u\xi_n)(\rho^{-1})\zeta_n(1)| \leqslant \frac{\lambda(n)}{1-\lambda(n)^2}4\pi\sqrt{2n+\frac{1}{2}}, \qquad \forall\rho,\ 1\leqslant\rho\leqslant 2.$$

The above inequalities then give

$$|B_n(\rho)| \leqslant \frac{\lambda(n)}{1-\lambda(n)^2}\left(8\pi\sqrt{2}+4\pi\right)\sqrt{2n+\frac{1}{2}}. \tag{169}$$

We thus obtain

Lemma F.1 *(i) The series* (99) *of Proposition 5.3 is convergent and the remainder (after replacing the infinite sum by the sum of the first* N *terms) is majored as follows*

$$|Q\epsilon(\rho)-\sum_0^N \frac{\lambda(k)}{\sqrt{1-\lambda(k)^2}}T_k(\rho)| \leqslant \sum_{N+1}^{\infty}\frac{2^{2n+2}\pi^{2n+\frac{3}{2}}p(n)((2n)!)^2}{(4n)!\Gamma\left(2n+\frac{3}{2}\right)} \tag{170}$$

where $p(n)=16n^2+8(1+3\pi)n+(4+\sqrt{2})\sqrt{4n+1}+32\pi^2+24\pi+2.$
(ii) For $N=10$*, the remainder is less than* 2.366×10^{-12} *for any* $\rho\in[1,2]$*:*

$$|Q\epsilon(\rho)-\sum_0^{10}\frac{\lambda(k)}{\sqrt{1-\lambda(k)^2}}T_k(\rho)| \leqslant 2.366\times10^{-12}, \qquad \forall\rho\in[1,2]. \tag{171}$$

Proof. (i) follows from (168) and (169) which, together with (72), combine to yield for $n\geqslant 3$,

$$\left|\frac{\lambda(n)}{\sqrt{1-\lambda(n)^2}}T_n(\rho)\right| \leqslant 2\lambda(n)\left(|A_n(\rho)|+|B_n(\rho)|\right) \leqslant$$
$$\leqslant \frac{2^{2n+2}\pi^{2n+\frac{3}{2}}\left(16n^2+8(1+3\pi)n+(4+\sqrt{2})\sqrt{4n+1}+32\pi^2+24\pi+2\right)((2n)!)^2}{(4n)!\Gamma\left(2n+\frac{3}{2}\right)}$$

which gives (170).
(ii)To compute the upper bound of the right hand side of (170) for $N=10$, one splits the sum in two, using the simple estimate $p(n)\leqslant 120n^2$ for $n\geqslant 35$:

$$\frac{2^{2n+2}\pi^{2n+\frac{3}{2}}p(n)((2n)!)^2}{(4n)!\Gamma\left(2n+\frac{3}{2}\right)} \leqslant \frac{15\ 2^{2n+4}n^2\pi^{2n+\frac{1}{2}}((2n)!)^2}{(4n)!\Gamma\left(2n+\frac{3}{2}\right)}, \qquad \forall n\geqslant 35.$$

With ν_n the right hand side of this inequality, one obtains the relation

$$\nu_{n+1}/\nu_n = \frac{8\pi^2(n+1)^3(2n+1)}{n^2(4n+1)(4n+3)^2(4n+5)} = \frac{\pi^2}{16n^2}+\frac{\pi^2}{32n^3}+O\left(n^{-4}\right)$$

and $n^2\nu_{n+1}/\nu_n<1$ for all $n\geqslant 35$. One has $\nu_{35}\leqslant 5\times10^{-81}$, and thus using the trivial bound by the geometric series one gets

$$\sum_{35}^{\infty}\nu_n \leqslant \frac{1225}{1224}\nu_{35} \leqslant 10^{-80}.$$

One then simply computes the missing terms and they give

$$\sum_{11}^{34}\frac{2^{2n+2}\pi^{2n+\frac{3}{2}}p(n)((2n)!)^2}{(4n)!\Gamma\left(2n+\frac{3}{2}\right)} \sim 2.365\times10^{-12}$$

Thus combining the above inequalities we obtain (171). □

Remark F.2 *For completeness, we give a short proof of an improved form of* (167)*. As in [33] (Equation (3.26)) one has, using integration by parts, the identity, for $f \in C^\infty([-1,1],\mathbf{R})$, and $c = 2\pi$, using* (67)

$$\int_{-1}^{1} (\mathbf{W}f)^2(x)dx = \int_{-1}^{1} (1-x^2)^2|f''(x)|^2 dx + 2\int_{-1}^{1} (1-x^2)(1+c^2x^2)|f'(x)|^2 dx + \\ + c^2 \int_{-1}^{1} (c^2x^4 + 6x^2 - 2)|f(x)|^2 dx.$$

Applying this to $f = \xi_n$ and using $\mathbf{W}\xi_n = \chi_{2n}^{2\pi}\xi_n$ one gets

$$\int_{-1}^{1} (\xi_n''(x))^2(1-x^2)^2 dx \leqslant \int_{-1}^{1} (\mathbf{W}\xi_n)^2(x)dx + 2c^2 \int_{-1}^{1} \xi_n(x)^2 dx$$

providing the following improvement of (167)

$$\left(\int_{0}^{1} (\xi_n''(x))^2(1-x^2)^2 dx\right)^{\frac{1}{2}} \leqslant \sqrt{(\chi_{2n}^{2\pi})^2 + 2c^2} \leqslant 2n(2n+1) + (2\pi)^2(1+\sqrt{2}).$$

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