Trace formulae for Jacobi matrices

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Abstract

In this master thesis three problems are studied, in the area of functional analysis and operator theory. The main problem involves expanding the scattering coefficient analytically extended into the complex plane, into a Laurent series. The second problem involves calculating an integral of the transition coefficient, and the third problem involves finding the derivative of the absolutely continuous component of the spectral measure. Thereby we prove that the absolutely continuous spectrum fills the interval $[-2, 2]$ and there are no embedded eigenvalues on this interval.

Contents

1 Introduction

We will work in the Hilbert sequence space l^2, which here has element indices from $\mathbb{Z}$, so that an element is written $x = (\ldots, x_{-2}, x_{-1}, x_0, x_1, x_2, \ldots)$. The standard orthonormal basis in l^2 is denoted e_i, where $i \in \mathbb{Z}$. Thus,

$$(e_i)_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

Also, we use the notation (f, g) for the inner product in l^2, so that

$$(f, g) = \sum_{i=-\infty}^{\infty} f_i \overline{g}_i$$

The matrix of an operator A, with respect to the standard base, is the infinite matrix $M_A = [a_{ij}]$ where

$$a_{ij} = (Ae_j, e_i) \quad i, j \in \mathbb{Z}$$

Recall the well-known fact that A is uniquely defined by its matrix (if the base is fixed). If the matrix is tridiagonal it is called a *Jacobi matrix*.

For a triangular (normal, finite) matrix, the eigenvalues are the diagonal elements, and the determinant is the product of the diagonal elements, and in analogy with this, the determinant of an operator is the product of its eigenvalues. Similarly, any relation involving sums of eigenvalues of an operator is regarded as a *trace formula*.

In this setting we will study three problems. The main problem involves finding a trace formula, and the second uses the trace formula to calculate some interesting Riemann integrals. Finally, the third problem also uses results from the solution of the main problem, and also involves an integral.

2 Main problem

2.1 Formulation

The main problem that we will study is formulated as follows. Let S be the shift operator in l^2, which shifts all elements of a vector one step to the right, so $(Sx)_j = x_{j-1}$ for $j \in \mathbb{Z}$. Let V be the operator which multiplies a given vector elementwise with the vector v, where $v_0 = q \in \mathbb{R} \setminus \{0\}$ and $v_j = 0$ for $j \neq 0$. That is, we have that

$$(Vx)_j = \begin{cases} qx_0 & j = 0 \\ 0 & j \neq 0 \end{cases}$$

Thus, the matrix $M_V = [a_{ij}]$ has zeros everywhere, except $a_{00} = q$, and is a Jacobi matrix. Now, recall that S^* is the adjoint operator to S. Let $H = S + S^*$ and define the complex-valued function $a(k) = \det(I + V(H - zI)^{-1})$ where

$z = k + 1/k$, $z \in \rho(H)$ and I is the identity operator. The function $a(k)$ is called the *scattering coefficient*.

Now, the problem is to expand $\log a(k)$ in a Laurent series when $|k|$ is very large.

2.2 Solution

2.2.1 Initial observations

Note that S^* is the operator which shifts all elements one step to the left, so $(S^*x)_j = x_{j+1}$. Thus, the matrix M_H has zeros everywhere, except at the first super- and subdiagonals, which consist of ones, and thus M_H is a Jacobi matrix. Also note that, because of the symmetry of z, we can let $|k|$ be very small instead of very large. Just substitute $k' = 1/k$ and note that $z = k' + 1/k'$, which is the same formula as the original, and $|k'| \to \infty$ as $|k| \to 0$.

Thus, we will assume $|k| < 1$ and we want to find an expression for $a(k)$.

2.2.2 Calculating eigenvalues

We want to find all eigenvalues of $I + V(H - zI)^{-1}$, so we want to solve the equation

$$(I + V(H - zI)^{-1})f = \lambda f \tag{1}$$

which is directly simplified to

$$V(H - zI)^{-1}f = (\lambda - 1)f \tag{2}$$

where $f \in l^2$ and $\lambda \in \mathbb{C}$.

The left-hand side of (2) has the form ce_0, where

$$c = q((H - zI)^{-1}f, e_0) \tag{3}$$

so the only possible eigenvector has the form $f = de_0$. In that case, because of the homogeneity of the inner product, we have

$$dq((H - zI)^{-1}e_0, e_0)e_0 = d(\lambda - 1)e_0 \tag{4}$$

and thus d is unnecessary and $f = e_0$ is the unique eigenvector, corresponding to the single eigenvalue λ given by

$$\lambda = 1 + q((H - zI)^{-1}e_0, e_0) \tag{5}$$

To calculate the inner product, we must solve the equation

$$u = (H - zI)^{-1}e_0 \tag{6}$$

for $u \in l^2$. This is equivalent to solving

$$(H - zI)u = Su + S^*u - zu = e_0 \tag{7}$$

Recalling the definition of S and its adjoint, this is just the following linear difference equation

$$u_{i+1} + u_{i-1} - zu_i = \begin{cases} 1 & i = 0 \\ 0 & i \neq 0 \end{cases} \tag{8}$$

2.2.3 Solving linear difference equation

So now we have a linear difference equation, or recursive equation, given by (8). We change the formulation, to equate it more with the theory of difference equations, so that we want to find $u(n)$ for all $n \in \mathbb{Z}$, that satisfies

$$u(n+1) + u(n-1) - zu(n) = \delta_{0,n} \tag{9}$$

where $\delta_{i,j}$ is the Kronecker symbol. Also, because we live in l^2, we must have that $|u(n)| \to 0$ as $n \to \pm\infty$. From (9), we have three cases, as follows

$$\begin{aligned} u(n+2) - zu(n+1) + u(n) = 0 \quad & n > 0 & (10)\\ u(m+2) - zu(m+1) + u(m) = 0 \quad & -m = n < 0 & (11)\\ u(1) + u(-1) + zu(0) = 1 \quad & n = 0 & (12) \end{aligned}$$

We first analyse (10). The characteristic equation is $r^2 - zr + 1 = 0$, with solutions

$$r = \frac{z \pm \sqrt{z^2-4}}{2} \tag{13}$$

Thus, the general solution to (10) is

$$u(n) = c_1 \left(\frac{z + \sqrt{z^2-4}}{2} \right)^n + c_2 \left(\frac{z - \sqrt{z^2-4}}{2} \right)^n \tag{14}$$

where c_1 and c_2 are arbitrary complex numbers. Recalling the definition of $z = k + 1/k$, we have that $z^2 - 4 = k^2 + 1/k^2 - 2 = (k - 1/k)^2$ and so (14) simplifies to

$$u(n) = c_1 k^n + c_2 k^{-n} \tag{15}$$

As mentioned, we must have that $|u(n)| \to 0$ as $n \to \pm\infty$. In this case, only the positive limit is interesting, and this forces $c_2 = 0$, because we are assuming $|k| < 1$, since we are interested in what happens when $|k|$ is very small. We thus get our particular solution to (10) as

$$u(n) = C_1 k^n \tag{16}$$

where $C_1 \in \mathbb{C}$.

To analyse the case given by (11), we note that the calculations are the same as in the analysis of (10), up to (15). In this case we are interested in the limit as n goes to $-\infty$, and this forces $c_1 = 0$. We thus get our particular solution to (11) as

$$u(n) = C_2 k^{-n} \tag{17}$$

where $C_2 \in \mathbb{C}$.

The case given by (12) only involves finding the value of $u(0)$. From (9), we get three equations involving $u(0)$, as follows

$$\begin{aligned} u(1) + u(-1) - zu(0) &= 1 & (18)\\ u(2) + u(0) - zu(1) &= 0 & (19)\\ u(0) + u(-2) - zu(-1) &= 0 & (20) \end{aligned}$$

Using (16) and (17) this becomes the following system of linear equations in three unknowns

$$C_1k + C_2k - zu(0) = 1 \tag{21}$$
$$C_1k^2 + u(0) - zC_1k = 0 \tag{22}$$
$$u(0) + C_2k^2 - zC_2k = 0 \tag{23}$$

Expanding z in (22), gives $u(0) = C_1$, and doing the same in (23) gives $u(0) = C_2$. Thus, (21) gives

$$u(0) = \frac{k}{k^2 - 1} \tag{24}$$

Tracing our steps, we see that from (5), the only interesting value of $u(n)$ is $u(0)$. Because there is a unique solution (24), our function $a(k)$ is just the unique eigenvalue given by (5), so we finally have

$$a(k) = 1 + q\frac{k}{k^2 - 1} \tag{25}$$

2.2.4 Expanding in a Laurent series

Now we should expand $f(k) = \log a(k)$ in a Laurent series, when $|k|$ is very large, but from the observation in section 2.2.1, we can instead find the Taylor expansion valid when $|k|$ is close to zero, ie. the Maclaurin expansion.

First, we analyse the analyticity of $f(k)$, to determine if expansion is possible at all. From (25) we have

$$a(k) = \frac{k^2 + qk - 1}{k^2 - 1} \tag{26}$$

which have simple poles in $k = \pm 1$ and roots in

$$k = \frac{q \pm \sqrt{q^2 - 4}}{2} \tag{27}$$

Exactly one of the roots is inside the disc $|k| < 1$, which one depending on the sign of q. Let β_1 and β_2 be the roots, with $|\beta_1| < 1$. The derivation of (25) assumed that $|k| < 1$, and if we instead assume $|k| > 1$, we get

$$a(k) = \frac{k^2 - qk - 1}{k^2 - 1} \tag{28}$$

with roots in $k = \gamma_{1,2} = -\beta_{2,1}$.

Both the poles and the roots of $a(k)$ are poles of $f(k)$. If we choose the positive real line as branch cut for the complex logarithm, then we know that $f(k)$ is analytic at all points k except those that satisfy $\operatorname{Im} k = 0$ and $\operatorname{Re} k \geq 0$.

Thus, we will use $a(k)$ in the form given by (26). In this form, $f(k)$ is analytic on the disc $k < |\beta|$ where β is the root of $a(k)$ inside the unit disc, so it really is possible to expand $f(k)$ into a series.

The Maclaurin expansion of $f(k) = \log a(k)$ is a function $T(x)$ on the form

$$T(x) = \sum_{n=0}^{\infty} c_n x^n \tag{29}$$

where the coefficients have the form $c_n = \frac{f^{(n)}(0)}{n!}$.

Lemma 1 *Let* $b(k) = (k^2 + qk - 1)(k^2 - 1)$*,* $g_1(k) = b'(k)$ *and*

$$g_n(k) = g'_{n-1}(k)(b(k))^{2^{n-2}} - g_{n-1}(k)2^{n-2}(b(k))^{2^{n-2}-1}b'(k) \tag{30}$$

for $n > 1$*. Then, for* $n > 1$*, we have*

$$f^{(n)}(k) = \frac{g'_{n-1}(k)b(k) - 2^{n-2}g_{n-1}(k)b'(k)}{(b(k))^{2^{n-2}+1}} \tag{31}$$

Proof. We have that $f(k) = \log a(k)$ and that

$$f'(k) = \frac{a'(k)}{a(k)} = \frac{b'(k)}{b(k)} = \frac{\alpha_1(k)}{\beta_1(k)} \tag{32}$$

where $\alpha_1(k) = g_1(k)$ and $\beta_1(k) = b(k)$. Inductively, if we assume

$$f^{(n)}(k) = \frac{\alpha_n(k)}{\beta_n(k)} \tag{33}$$

then

$$f^{(n+1)}(k) = \frac{\alpha'_n(k)\beta_n(k) - \beta'_n(k)\alpha_n(k)}{(\beta_n(k))^2} = \frac{\alpha_{n+1}(k)}{\beta_{n+1}(k)} \tag{34}$$

where $\beta_{n+1}(k) = (\beta_n(k))^2$ and $\alpha_{n+1}(k) = \alpha'_n(k)\beta_n(k) - \beta'_n(k)\alpha_n(k)$, which defines their recurrencies. The recurrence for $\beta_n(k)$ is immediately solved into

$$\beta_n(k) = (\beta_1(k))^{2^{n-1}} \tag{35}$$

If we combine (35) and (34) we get, for $n > 1$,

$$f^{(n)}(k) = \frac{\alpha'_{n-1}(k)(\beta_1(k))^{2^{n-2}} - 2^{n-2}(\beta_1(k))^{2^{n-2}-1}\beta'_1(k)\alpha_{n-1}(k)}{(\beta_1(k))^{2^{n-1}}} \tag{36}$$

which is simplified into

$$f^{(n)}(k) = \frac{\alpha'_{n-1}(k)\beta_1(k) - 2^{n-2}\beta'_1(k)\alpha_{n-1}(k)}{(\beta_1(k))^{2^{n-2}+1}} \tag{37}$$

Note that $\alpha_n = g_n$ for all $n \geq 1$, so the lemma follows from (37). □

Lemma 2 *Let* $d_n^i = g_n^{(i)}(0)$, *where* $g_n(k)$ *is defined as in lemma 1. The numbers* d_n^i *satisfy the recurrence*

$$d_n^i = \begin{cases} b^{(i)}(0) & n = 1 \\ \sum_{j=0}^{i} \binom{i}{j} \left(d_{n-1}^{i+1-j} e_j - d_{n-1}^{i-j} e_{j+1} \right) & n > 1 \end{cases} \tag{38}$$

where the numbers e_m *are given by*

$$e_m = \sum \frac{m!}{k_1! \cdot k_2! \cdot k_3! \cdot k_4!} \frac{(2^n - 2)!}{(2^n - 2 - k)!} q^{k_1+k_3} 2^{k_2} (-1)^{k_2+k_3} \tag{39}$$

where $k = k_1 + k_2 + k_3 + k_4$ *and the sum is taken over all natural numbers* k_1, k_2, k_3, k_4 *such that*

$$k_1 + 2k_2 + 3k_3 + 4k_4 = m$$

Proof. Applying Leibniz Identity, the differentiation rule for a product of two functions, to both terms of (30), gives us

$$g_n^{(i)}(k) = \left[\sum_{j=0}^{i} \binom{i}{j} g_{n-1}^{(i+1-j)}(k) h^{(j)}(k) \right] - \left[\sum_{j=0}^{i} \binom{i}{j} g_{n-1}^{(i-j)}(k) h^{(j+1)}(k) \right] \tag{40}$$

where $h(k) = (b(k))^{2^{n-2}}$. If we let $e_m = h^{(m)}(0)$ we get (38). On the other hand, applying Faá di Bruno's formula, the differentiation rule for a composition of two functions, to $h(k)$, and recalling that $b^{(i)}(k) = 0$ for $i > 4$, gives (39). □

Theorem 1 *The coefficients* c_n *in* (29) *can be calculated as*

$$c_n = \begin{cases} 0 & n = 0 \\ -q & n = 1 \\ \frac{1}{n!} \left(d_{n-1}^1 + 2^{n-2} q d_{n-1}^0 \right) & n > 1 \end{cases} \tag{41}$$

where the numbers d_n^i *are defined as in lemma 2.*

Proof. We have that $a(0) = 1$, $b(0) = 1$ and $b'(0) = -q$, from which it follows that $c_0 = 0$ and $c_1 = -q$, because of (32). For $n > 1$ the theorem follows from (31). □

3 Second problem

3.1 Formulation

Here, we want to calculate integrals involving the *transition coefficient*, which with our definitions is $1/a(k)$. To be more specific, we will consider integrals of the form

$$\int_{-\pi}^{\pi} \log \left(|a(e^{i\theta})| \right) w(\theta)\, d\theta \tag{42}$$

for different weight functions $w(\theta)$. We will study the case $w(\theta) = \sin^2 \theta$. The complex logarithm is defined using the principal branch, with the the negative real line as branch cut. It does not matter if we define $a(k)$ according to (28) or (26), since we will not use the explicit formulas for the roots of $a(k)$.

3.2 Solution

We calculate the integral by using the substitution $k = e^{i\theta}$, $d\theta = \frac{dk}{ik}$. Because $\sin\theta = \frac{e^{i\theta}-e^{-i\theta}}{2i}$, (42) transforms to

$$\frac{i}{4}\int_{\mathcal{C}} \frac{\log\left(|a(k)|\right)(k^4 - 2k^2 + 1)}{k^3}\, dk \tag{43}$$

where $\mathcal{C}$ is the unit circle in the complex plane.

We could use the Cauchy Integral Formula to calculate this integral, if the numerator in the integrand was analytic on and inside $\mathcal{C}$. Unfortunately, in (43) this is not the case, because from section 2.2.4 we know that $a(k)$ has poles and roots on and inside $\mathcal{C}$.

3.2.1 Blaschke product

The function $a(k)$ has two roots, where exactly one is inside $\mathcal{C}$. Let β be the root that is inside, and introduce the *Blaschke product* $B(k)$, defined as

$$B(k) = -\frac{k-\beta}{1-k\beta}\frac{\beta}{|\beta|} \tag{44}$$

Because $B(k)$ also has a root at β, we will see that the quotient $\frac{a(k)}{B(k)}$ is analytic inside $\mathcal{C}$. The introduction of $B(k)$ is also motivated by the following convenient properties.

Proposition 1 *If $k = e^{i\theta}$, then $|B(k)| = 1$.*

Proof. When $k = e^{i\theta}$, we have

$$|B(k)| = \left|\frac{e^{i\theta}-\beta}{1-e^{i\theta}\beta}\frac{\beta}{|\beta|}\right| = \left|\frac{e^{i\theta}-\beta}{e^{i\theta}(e^{-i\theta}-\beta)}\right| \tag{45}$$

Because cosine is an even function, $|e^{i\theta}-\beta| = |e^{-i\theta}-\beta|$, and the result follows. □

The following corollary follows immediately.

Corollary 1 *The integral in* (43) *equals the following integral:*

$$\frac{i}{4}\int_{\mathcal{C}} \frac{\log\left(\left|\frac{a(k)}{B(k)}\right|\right)(k^4 - 2k^2 + 1)}{k^3}\, dk \tag{46}$$

Proposition 2 *If $k = e^{i\theta}$, then $\operatorname{Im}\log\frac{a(k)}{B(k)}$ is an odd function of θ.*

Proof. Let $\beta' = -1/\beta$ be the root of $a(k)$ that lies outside of $\mathcal{C}$. Then we have

$$\begin{aligned} \frac{a(k)}{B(k)} &= \\ &= -\frac{(k-\beta)(k-\beta')}{(k-1)(k+1)} \frac{1-k\beta}{k-\beta} \frac{|\beta|}{\beta} && (47) \\ &= |\beta|(k-1/\beta)\frac{k-\beta'}{k^2-1} && (48) \\ &= |\beta|\frac{k^2-\beta'^2}{k^2-1} && (49) \end{aligned}$$

If θ changes to $-\theta$, then k changes to $\overline{k}$. Now we have

$$\operatorname{Im}\log\frac{a(k)}{B(k)} = \arg\frac{a(k)}{B(k)} = -\arg\overline{\left(\frac{a(k)}{B(k)}\right)} \tag{50}$$

and it follows from (49) that

$$\frac{a(\overline{k})}{B(\overline{k})} = |\beta|\frac{\overline{k}\cdot\overline{k}-\beta'^2}{\overline{k}\cdot\overline{k}-1} = |\beta|\overline{\frac{k\cdot k-\beta'^2}{k\cdot k-1}} = \overline{\left(\frac{a(k)}{B(k)}\right)} \tag{51}$$

Thus, from (50) we have

$$\operatorname{Im}\log\frac{a(k)}{B(k)} = -\operatorname{Im}\log\frac{a(\overline{k})}{B(\overline{k})} \tag{52}$$

and the proof is completed.□

Corollary 2 *The integral in* (46) *equals the following integral:*

$$\frac{i}{4}\int_{\mathcal{C}} \frac{\log\left(\frac{a(k)}{B(k)}\right)(k^4-2k^2+1)}{k^3}\,dk \tag{53}$$

Proof. We have that

$$\begin{aligned} \frac{i}{4}\int_{\mathcal{C}} \frac{\log\left(\frac{a(k)}{B(k)}\right)(k^4-2k^2+1)}{k^3}\,dk &= && (54) \\ = \frac{i}{4}\int_{\mathcal{C}} \frac{\log\left(\left|\frac{a(k)}{B(k)}\right|\right)(k^4-2k^2+1)}{k^3}\,dk && (55) \\ + \ i\int_{-\pi}^{\pi} \arg\left(\frac{a(e^{i\theta})}{B(e^{i\theta})}\right)\sin^2\theta\,d\theta && (56) \end{aligned}$$

and the second integral is zero, because the integrand is odd. □

3.2.2 Analyticity

We now investigate the analyticity of the numerator of the integrand in (53). The weight function is analytic, so we need only check where $\log \frac{a(k)}{B(k)}$ is analytic, which is everywhere except at all points k satisfying $\mathrm{Re}\, \frac{a(k)}{B(k)} \leq 0$ and $\mathrm{Im}\, \frac{a(k)}{B(k)} = 0$. Letting $k = x + iy$ in (49), where $x, y \in \mathbb{R}$, we get

$$\begin{aligned} \frac{a(k)}{B(k)} &= \\ &= |\beta| \frac{(x^2 - y^2 + 2ixy - \beta'^2)(x^2 - y^2 - 2ixy - 1)}{(x^2 - y^2 - 1)^2 + 4y^2} && (57) \\ &= |\beta| \frac{x^4 + 2x^2y^2 + y^4 + (1 + \beta'^2)(y^2 - x^2) - 2ixy(1 - \beta'^2) + \beta'^2}{(x^2 - y^2 - 1)^2 + 4y^2} && (58) \end{aligned}$$

from which it follows that the imaginary part of $\frac{a(k)}{B(k)}$ is zero iff $x = 0$ or $y = 0$. If $x = 0$, then the real part is

$$|\beta| \frac{y^4 + (1 + \beta'^2)y^2 + \beta'^2}{(y^2 - 1)^2 + 4y^2} \tag{59}$$

which is never less than or equal to 0. On the other hand, if $y = 0$, then the real part is

$$|\beta| \frac{x^4 - (1 + \beta'^2)x^2 + \beta'^2}{(x^2 - 1)^2 + 4x^2} \tag{60}$$

which is less than or equal to 0 on the line segments $-\beta'^2 \leq x \leq -1$ and $1 \leq x \leq \beta'^2$. That is, only the two points $k = \pm 1$ are dangerous to us, and unfortunately they are right on our integration curve $\mathcal{C}$.

3.2.3 Integration curves

Because the integrand in (53) is not analytic at the points $k = \pm 1$, we instead calculate the following integral:

$$\lim_{\epsilon \to 0} \left[\int_{-\pi+\epsilon}^{-\epsilon} \log \left(\frac{a(e^{i\theta})}{B(e^{i\theta})} \right) \sin^2 \theta \, d\theta + \int_{\epsilon}^{\pi-\epsilon} \log \left(\frac{a(e^{i\theta})}{B(e^{i\theta})} \right) \sin^2 \theta \, d\theta \right] \tag{61}$$

but we would like to integrate around a simple closed curve, to be able to use the Cauchy Integral Formula. Therefore, let the curve $\mathcal{D}$ be the closed curve around origo, consisting of the four parts $\mathcal{D}_1, \ldots, \mathcal{D}_4$, defined as

$$\begin{aligned} \mathcal{D}_1 &= \{k \mid k = e^{i\theta}, \epsilon \leq \theta \leq \pi - \epsilon\} && (62) \\ \mathcal{D}_2 &= \{k \mid k = \epsilon e^{i\theta} - 1, -\alpha_1 \leq \theta \leq \alpha_1\} && (63) \\ \mathcal{D}_3 &= \{k \mid k = e^{i\theta}, -\pi + \epsilon \leq \theta \leq -\epsilon\} && (64) \\ \mathcal{D}_4 &= \{k \mid k = \epsilon e^{i\theta} + 1, -\alpha_2 \leq \theta \leq \alpha_2\} && (65) \end{aligned}$$

where α_1 is the angle, with respect to $k=-1$, of the crossing between $\mathcal{D}_1$ and $\mathcal{D}_2$, and α_2 is the angle, with respect to $k=1$, of the crossing between $\mathcal{D}_1$ and $\mathcal{D}_4$. We can determine α_1 and α_2 by noting that

$$e^{i(\pi-\epsilon)} = \epsilon e^{i\alpha_1} - 1 \tag{66}$$

$$e^{i\epsilon} = \epsilon e^{i\alpha_2} + 1 \tag{67}$$

from which it follows that

$$\alpha_1 = \arg \frac{e^{i(\pi-\epsilon)}+1}{\epsilon} \tag{68}$$

$$\alpha_2 = \arg \frac{e^{i\epsilon}-1}{\epsilon} \tag{69}$$

Now, consider the following integral around $\mathcal{D}$, where we move counterclockwise around $\mathcal{D}_1$ and $\mathcal{D}_3$, and clockwise around $\mathcal{D}_2$ and $\mathcal{D}_4$:

$$\frac{i}{4}\int_{\mathcal{D}} \frac{\log\left(\frac{a(k)}{B(k)}\right)(k^4-2k^2+1)}{k^3}\,dk = \tag{70}$$

$$= \lim_{\epsilon\to 0} \int_{-\pi+\epsilon}^{-\epsilon} \log\left(\frac{a(e^{i\theta})}{B(e^{i\theta})}\right)\sin^2\theta\,d\theta \tag{71}$$

$$+ \int_{-\alpha_1}^{\alpha_1} \log\left(\frac{a(\epsilon e^{-i\theta}-1)}{B(\epsilon e^{-i\theta}-1)}\right)\sin^2\theta\,d\theta \tag{72}$$

$$+ \int_{-\alpha_2}^{\alpha_2} \log\left(\frac{a(\epsilon e^{-i\theta}+1)}{B(\epsilon e^{-i\theta}+1)}\right)\sin^2\theta\,d\theta \tag{73}$$

$$+ \int_{\epsilon}^{\pi-\epsilon} \log\left(\frac{a(e^{i\theta})}{B(e^{i\theta})}\right)\sin^2\theta\,d\theta \tag{74}$$

If the integrals in (72) and (73) goes to 0 as ϵ goes to 0, then the integral in (70) equals the integral in (61), and we will show that it is indeed the case.

Proposition 3 *The integrals in* (72) *and* (73) *goes to 0 as* ϵ *goes to 0*

Proof. We will use the so called ML inequality, and analyse (72) only, since the other case is similar. The integration curve is an arc of a circle with radius ϵ, so we have

$$L = 2\epsilon\alpha_1 \tag{75}$$

which goes to 0 as ϵ goes to zero, because $\lim_{\epsilon\to 0}\alpha_1 = \pi/2$. On the other hand, using (49) we have

$$\left|\frac{a(\epsilon e^{-i\theta}-1)}{B(\epsilon e^{-i\theta}-1)}\right| = \tag{76}$$

$$= |\beta|\left|\frac{\epsilon^2 e^{-2i\theta}+1-2\epsilon e^{-i\theta}-\beta'^2}{\epsilon^2 e^{-2i\theta}-2\epsilon e^{-i\theta}}\right| \tag{77}$$

$$\leq |\beta|\frac{\epsilon^2+1+2\epsilon+\beta'^2}{\epsilon^2-2\epsilon} \tag{78}$$

which goes to ∞ as ϵ goes to 0. This gives us

$$\left|\log\left(\frac{a(\epsilon e^{-i\theta}-1)}{B(\epsilon e^{-i\theta}-1)}\right)\sin^2\theta\right| \leq \tag{79}$$

$$\leq \sqrt{\left(\log\left|\frac{a(\epsilon e^{-i\theta}-1)}{B(\epsilon e^{-i\theta}-1)}\right|\right)^2+\left(\arg\frac{a(\epsilon e^{-i\theta}-1)}{B(\epsilon e^{-i\theta}-1)}\right)^2} \tag{80}$$

$$\leq \sqrt{\pi^2+\left(\log\left||\beta|\frac{\epsilon^2+1+2\epsilon+\beta'^2}{\epsilon^2-2\epsilon}\right|\right)^2} = M \tag{81}$$

which goes to ∞ as ϵ goes to 0. But because of the logarithm in M, it is certainly true that

$$\lim_{\epsilon\to 0} ML = 0 \tag{82}$$

and the proof is completed. □

3.2.4 Final calculation

Thus, the integral in (70) is taken around a simple closed curve, and the integrand is analytic on and inside the curve, except at origo. The Cauchy Integral Formula then gives us

$$\frac{i}{4}\int_{\mathcal{D}} \frac{\log\left(\frac{a(k)}{B(k)}\right)(k^4-2k^2+1)}{k^3}\,dk = \tag{83}$$

$$= -\frac{\pi}{4}\frac{d^2}{dk^2}\left(\log\left(\frac{a(k)}{B(k)}\right)(k^4-2k^2+1)\right)\Bigg|_{k=0} \tag{84}$$

$$= \frac{\pi}{2\beta'^2}(1-\beta'^2+2\log(|\beta'|)\beta'^2) \tag{85}$$

$$= \frac{\pi}{2}(\beta^2-1+2\log(|\beta'|)) \tag{86}$$

Thus, we have calculated the integral, and the argument can easily be extended to other weight functions. For weights that are analytic and even, with absolute value bounded by a constant, there is not really any change at all, except in the final calculation. An example is $w(\theta)=1$, in which case the value of the integral is the same, except for the logarithm term in (86), which disappears.

4 Final problem

4.1 Formulation

Recall the operators S and V, defined in section 2.1. Redefine the operator H so that it contains a small perturbation, as follows:

$$H = S + S^* + V \tag{87}$$

Now H still admits a Jacobi matrix, with a single nonzero element in the main diagonal, and the first super- and subdiagonals consisting of ones. Define the function $F(z)$ as

$$F(z) = \big((H - zI)^{-1}e_0, e_0\big) \tag{88}$$

where $z \in \rho(H)$. Let h be the eigenvector to H such that $\|h\| = 1$, let E be the corresponding eigenvalue and let $c = |(h, e_0)|^2$. Now the problem is to find a real-valued function $f(t)$ such that

$$\frac{c}{E - z} + \int_{-2}^{2} \frac{f(t)}{t - z}\, dt = F(z) \tag{89}$$

In other words, we want to express the spectral measure $d\mu$ of the Cauchy integral for $F(z)$ as $f(t)\,dt$, and thereby prove that the absolutely continous spectrum of H can be defined on the whole interval $[-2, 2]$.

4.2 Solution

As before, without loss of generality, let $z = k + 1/k$, where $|k| < 1$. Notice that the function $F(z)$ is the same as the value $u(0)$ from (24) except that H is now different. Anyway, we can use the same method as in sections 2.2.2 and 2.2.3 to find $F(z)$. Thus, we are led to consider the analogue of (7),

$$(H - zI)u = Su + S^*u + Vu - zu = e_0 \tag{90}$$

which leads to the analogue of (9)

$$u(n+1) + u(n-1) - zu(n) = (1 - qu(0))\delta_{0,n} \tag{91}$$

As before, we assume $|k| < 1$, and the analogue of (21) to (23) will be

$$C_1k + C_2k - zu(0) = 1 - qu(0) \tag{92}$$

$$C_1k^2 + u(0) - zC_1k = 0 \tag{93}$$

$$u(0) + C_2k^2 - zC_2k = 0 \tag{94}$$

which gives us

$$F(z) = \frac{1}{k - 1/k + q} = \frac{k}{k^2 + qk - 1} \tag{95}$$

Notice that the poles of $F(z)$ are the roots of $a(k)$ defined in (26).

4.2.1 Finding E and c

To find the eigenvalue E and the the value c, we need to solve the eigenvalue equation

$$Hf = Sf + S^*f + Vf = Ef \tag{96}$$

which, as before, leads to the difference equation

$$f(n+1) + f(n-1) - Ef(n) = -qf(0)\delta_{0,n} \tag{97}$$

If we let $E = \alpha + 1/\alpha$, where $|\alpha| < 1$, then this equation is analogous to (91). We use the same method as before, and obtain that for $n > 0$, the eigenvector satisfies

$$f = C_1 \alpha^n \tag{98}$$

and for $n < 0$ it satisfies

$$f = C_1 \alpha^{-n} \tag{99}$$

Thus, we are led to the analogue of (92) to (94)

$$C_1\alpha + C_2\alpha - Ef(0) = -qf(0) \tag{100}$$
$$C_1\alpha^2 + f(0) - EC_1\alpha = 0 \tag{101}$$
$$f(0) + C_2\alpha^2 - EC_2\alpha = 0 \tag{102}$$

We do not get an expression for $f(0)$ this time, because it cancels in (100), but instead we get an equation for α, namely

$$\alpha^2 + q\alpha - 1 = 0 \tag{103}$$

which has the same roots as $a(k)$ defined in (26) (the poles of $F(z)$). If we once again let β be the root inside the unit disc, then $\alpha = \beta$ because α is also defined to be inside the unit disc. Thus, we have found the eigenvalue

$$E = \beta + 1/\beta \tag{104}$$

From (100) to (102) we also get $C_1 = C_2 = f(0)$, so the eigenvector is

$$f = f(0)\beta^{|n|} \tag{105}$$

Notice that the zero coordinate is free, but we are interested in the eigenvector h with unit norm, so we have

$$1 = \sum_{n\in\mathbb{Z}} |h_n|^2 = 2\sum_{n=0}^{\infty} |h_0|^2\beta^{2n} - |h_0|^2 = 2\frac{|h_0|^2}{1-\beta^2} - |h_0|^2 \tag{106}$$

from which it follows that

$$c = |h_0|^2 = \left(\frac{1-\beta^2}{1+\beta^2}\right) \tag{107}$$

4.2.2 Finding f(t)

To find the function $f(t)$, we make use of a well-known theorem from Mathematical Physics, which we state without proof.

Theorem 2 *Let $F(z)$ and $f(t)$ be defined as in section 4.1. If $\lambda \in \mathbb{R}$ and $\epsilon \in \mathbb{R}$, then*

$$\lim_{\epsilon \to 0} \mathrm{Im} F(\lambda + i\epsilon) = \pi f(\lambda) \tag{108}$$

So, if we let $k = re^{i\theta}$, where $-\pi \leq \theta \leq 0$, then

$$z = \left(r + \frac{1}{r}\right) \cos\theta + i \left(r - \frac{1}{r}\right) \sin\theta \tag{109}$$

If now $r \to 1-$, then $\epsilon = \sin\theta \left(r - \frac{1}{r}\right) \to 0+$, and $\lambda = \cos\theta \left(r + \frac{1}{r}\right) \to 2\cos\theta$.

Expressing $F(z)$ in this polar form, we get

$$F(z) = \tag{110}$$

$$= \frac{re^{i\theta}}{r^2 e^{2i\theta} + qre^{i\theta} - 1} \tag{111}$$

$$= \frac{r^3 e^{-i\theta} + qr^2 - re^{i\theta}}{\left(r^2 \cos 2\theta + qr\cos\theta - 1\right)^2 + \left(r^2 \sin 2\theta + qr\sin\theta\right)^2} \tag{112}$$

Taking the imaginary part and letting r turn to 1, we get

$$\pi f(2\cos\theta) = \tag{113}$$

$$= \frac{-2\sin\theta}{\left(\cos 2\theta + q\cos\theta - 1\right)^2 + \left(\sin 2\theta + q\sin\theta\right)^2} \tag{114}$$

$$= \frac{-2\sin\theta}{2 + q^2 - 2\cos 2\theta + 2q\left(\sin 2\theta \sin\theta + \cos 2\theta \cos\theta - \cos\theta\right)} \tag{115}$$

$$= \frac{-2\sin\theta}{q^2 + 2\left(1 - \cos 2\theta + q\left(\sin 2\theta \sin\theta + \cos 2\theta\cos\theta - \cos\theta\right)\right)} \tag{116}$$

$$= \frac{-2\sin\theta}{q^2 + 4\left(\sin^2\theta + q\left(\cos\theta\sin^2\theta - \cos\theta\sin^2\theta\right)\right)} \tag{117}$$

$$= \frac{-2\sin\theta}{q^2 + 4\sin^2\theta} \tag{118}$$

Thus, we have found the integrand in (89) and so it is possible to express the spectral measure as $f(t)\,dt$, which is what we wanted to prove. Again, note that $-\pi \leq \theta \leq 0$ in (118), so the change of variables can be done correctly.