REFLECTIONLESS DIRAC OPERATORS AND MATRIX VALUED KREIN FUNCTIONS

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Dedicated with great pleasure to my mentor Barry Simon on the occasion of his 80th birthday. Happy Birthday, Barry!

ABSTRACT. This note presents a sharp bound on reflectionless Dirac operators.

1. INTRODUCTION

This brief note is a spin-off of [9]. Its goal is to prove Theorem 1.2 below. I originally tried to do this using the machinery of [9], but I then realized that the rather different methods from [1, 2] (developed, as it happens, by Barry and collaborators) work much better for this. Incidentally, similar remarks apply to some of the results of [4, 7]. So it seems to make sense to split this part off and present it separately here.

We consider Dirac equations

$$Jy'(x) + W(x)y(x) = -zy(x), \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{1.1}$$

and the associated operators $Ly = -Jy' - Wy$ on $L^2(\mathbb{R};\mathbb{C}^2)$. We assume that $W(x) \in \mathbb{R}^{2\times 2}$, $W(x) = W^t(x)$, $W \in L^1_{\text{loc}}(\mathbb{R})$. Then L is self-adjoint on its natural maximal domain

$$D(L) = \{y \in L^2(\mathbb{R};\mathbb{C}^2) : y \text{ absolutely continuous, } Jy' + Wy \in L^2\}.$$

The *Titchmarsh-Weyl m functions* may be defined as

$$m_\pm(z) = \pm y_\pm(0,z), \tag{1.2}$$

and here $z \in \mathbb{C}^+ = \{z \in \mathbb{C} : \operatorname{Im} z > 0\}$ and $y_\pm(x,z)$ denotes the unique, up to a constant factor, solution y of (1.1) that is square integrable on $\pm x > 0$. On the right-hand side of (1.2), we also use the convenient convention of identifying a vector $y = (y_1, y_2)^t \in \mathbb{C}^2$, $y \neq 0$, with the

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point $y_1/y_2 \in \mathbb{C}_\infty$ on the Riemann sphere. So $m_\pm$ take values in $\mathbb{C}_\infty$, and in fact these functions are *Herglotz functions,* that is, they map the upper half plane $\mathbb{C}^+$ holomorphically back to itself.

Clearly, each of $m_\pm$ refers to one half line only. Of course, both of them combined contain all the information on the whole line problem, so it must be possible to obtain a spectral representation of L from m_+ and m_-, and usually one proceeds as follows: combine $m_\pm$ into one matrix function

$$M(z) = \frac{-1}{m_+(z) + m_-(z)} \begin{pmatrix} -2m_+(z)m_-(z) & m_+(z) - m_-(z) \\ m_+(z) - m_-(z) & 2 \end{pmatrix}. \tag{1.3}$$

Then $M(z)$ is a *matrix valued Herglotz function,* that is, $M(z)$ is holomorphic on $\mathbb{C}^+$ and we still have $\operatorname{Im} M(z) > 0$ there, where we now define $\operatorname{Im} M = (M - M^*)/(2i)$. Please see [3] for a comprehensive discussion of matrix valued Herglotz functions in general.

Our function has the additional properties $M = M^t$, so maps into what is often called the *Siegel upper half space,* and $\det M(z) = -1$ for all $z \in \mathbb{C}^+$.

The M matrix provides a spectral representation of the Dirac operator L in the sense that L is unitarily equivalent to multiplication by the variable in $L^2(\mathbb{R}, d\rho)$ on the natural domain of this operator, and here the (matrix valued) *spectral measure* ρ is the measure from the Herglotz representation of M:

$$M(z) = A + Bz + \int_{-\infty}^{\infty} \left(\frac{1}{t-z} - \frac{t}{t^2+1} \right) d\rho(t)$$

The function $M(z)$ or, equivalently, the pair of functions $m_\pm(z)$ does not determine $W(x)$ uniquely; such a one-to-one correspondence can be obtained if W is suitably normalized, which can be done in various ways. In this paper, I will work with the $\operatorname{tr} W = 0$ normalization throughout. We can then write

$$W(x) = \begin{pmatrix} p(x) & q(x) \\ q(x) & -p(x) \end{pmatrix}. \tag{1.4}$$

These issues are discussed in more detail in the standard literature on the subject [5] and also in [10, Section 2], from a more abstract point of view.

We say that W or $L = L_W$ is *reflectionless* on a Borel set $A \subseteq \mathbb{R}$ if

$$m_+(t) = -\overline{m_-(t)} \tag{1.5}$$

for (Lebesgue) almost every $t \in A$. Here, $m_\pm(t) \equiv \lim_{y\to 0+} m_\pm(t+iy)$; these limits exist at almost all $t \in \mathbb{R}$. Reflectionless operators are important because they provide the basic building blocks for arbitrary operators with some absolutely continuous spectrum [6], [8, Ch. 7].

We also define, for closed sets $E \subseteq \mathbb{R}$,

$$\mathcal{R}(E) = \{W : L_W \text{ is reflectionless on } E\},$$
$$\mathcal{R}_0(E) = \{W \in \mathcal{R}(E) : \sigma(W) \subseteq E\}.$$

We will focus on *finite gap sets*

$$E = \mathbb{R} \setminus \bigcup_{j=1}^{n} (a_j, b_j), \tag{1.6}$$

with $a_1 < b_1 < a_2 < \ldots < b_n$, though the arguments below can also handle more general situations.

As in the scalar case, we can take the (matrix valued) logarithm of a matrix valued Herglotz function to obtain a new Herglotz function. We will review the details of the procedure in Section 2. The new function $\log M(z)$ has bounded imaginary part; in fact $0 < \text{Im } \log M(z) < \pi$ for a suitable choice of the logarithm, and this implies that the representing measure of $\log M(z)$ is purely absolutely continuous. Its matrix valued density $\xi(t) \in \mathbb{R}^{2\times 2}$, $0 \le \xi(t) \le 1$, is called the *Krein function* of $M(z)$. We have

$$\log M(z) = A + \int_{-\infty}^{\infty} \left(\frac{1}{t-z} - \frac{t}{t^2+1} \right) \xi(t)\, dt, \tag{1.7}$$

with $A = \text{Re } \log M(i) \in \mathbb{R}^{2\times 2}$, $A = A^t$.

The Krein function is a standard tool in the scalar case but it has not been used much for matrix valued Herglotz functions. It is easy to understand why this is so: if, let's say, $\xi(t) = 0$ or $\xi(t) = 1$ in the scalar setting, then obviously $m(t) = |m(t)|e^{i\pi\xi(t)}$ is real. However, if $\xi(t) = P$, a projection, in the matrix valued case, then we cannot automatically conclude that $M(t)$ is real even though $\xi(t)$ still has eigenvalues 0 and 1. More precisely, $M(t)$ will be real only if Re $\log M(t)$ commutes with P. So the converse of Proposition 1.1(c) below fails badly.

These issues might deserve further investigation in a general framework. I will not try to do this here. For my current purposes, the following straightforward properties of ξ will be sufficient.

Proposition 1.1. *(a) For any W, we have* $\text{tr}\, \xi(t) = 1$*, $t \in \mathbb{R}$.*
(b) [1] *$W \in \mathcal{R}(E)$ if and only if $\xi(t) = 1/2$ on $t \in E$.*
(c) For $t \notin \sigma(L)$, the Krein function is a projection:

$$\xi(t) = P_\alpha = \begin{pmatrix} \cos^2\alpha & \sin\alpha\cos\alpha \\ \sin\alpha\cos\alpha & \sin^2\alpha \end{pmatrix}$$

for some $\alpha = \alpha(t)$.

When combined with the methods of [1, 2], this will imply the following result. Recall here that if $W \in \mathcal{R}(E)$, $\operatorname{tr} W = 0$, then $W(x)$ is real analytic [10, Theorem 4.1], so it makes sense to evaluate this (matrix) function pointwise.

Theorem 1.2. *If* $W \in \mathcal{R}(E)$, $\operatorname{tr} W(x) = 0$, *with* E *as in* (1.6), *then*

$$\|W(x)\| \le \frac{1}{2}\sum_{j=1}^{n}(b_j - a_j). \tag{1.8}$$

Moreover, equality at a single $x_0 \in \mathbb{R}$ *implies that* $W \in \mathcal{R}_0(E)$, *and for any fixed* $x = x_0 \in \mathbb{R}$, *there are such* $W \in \mathcal{R}_0(E)$ *for which* (1.8) *holds with equality.*

Here, $\|W(x)\| = \sqrt{p^2(x) + q^2(x)}$ denotes the operator norm of $W(x)$.

If $n = 1$, so $E = \mathbb{R} \setminus (a, b)$, then $\|W(x)\| = (b - a)/2$ for all $W \in \mathcal{R}_0(E)$ and $x \in \mathbb{R}$, and each $W \in \mathcal{R}_0(E)$ is constant. This slightly strengthened version of Theorem 1.2 was obtained in [10], by different methods. The present proof is simpler.

However, if $n > 1$, a given $W \in \mathcal{R}_0(E)$ need not realize the bound (1.8) at any $x \in \mathbb{R}$ because orbits under the shift map $W(x) \mapsto W(x+a)$ need not be dense in $\mathcal{R}_0(E)$, and (of course) the map $W \mapsto \|W(0)\|$ is no longer constant on $\mathcal{R}_0(E)$ when $n > 1$.

2. Matrix valued logarithms and Krein functions

This section presents a quick review of material that can also be found in other sources such as [3] in one form or another, with a view towards our needs here.

For a complex number $w \in \Omega \equiv \mathbb{C} \setminus \{-iy : y \ge 0\}$, we define $\log w$ as the holomorphic function on this domain with $e^{\log w} = w$, $\log 1 = 0$. So in particular $0 < \operatorname{Im} \log w < \pi$ for $w \in \mathbb{C}^+$.

Having fixed this branch of the logarithm function, we then have available a well defined matrix $\log A$ for any $A \in \mathbb{C}^{2\times 2}$ with $\sigma(A) \subseteq \Omega$. It satisfies $(\log A)v = (\log \lambda)v$ if $Av = \lambda v$. This property determines $\log A$ if A is diagonalizable and could serve as the definition of $\log A$ in this case. The general case can be handled by approximation or a similar procedure, using the Jordan normal form. We have $e^{\log A} = A$, and here we define the matrix exponential as usual by its power series.

In particular, since $\operatorname{Im} M(z) > 0$, so $\sigma(M(z)) \subseteq \mathbb{C}^+$, we may use this matrix logarithm for $A = M(z)$. For such matrices A, with spectrum in the upper half plane, we can also compute $\log A$ as

$$\log A = \int_0^\infty \left(\frac{t}{t^2+1} - (t+A)^{-1} \right) dt, \tag{2.1}$$

as proposed in [3]. This formula works because the integral evaluates $\log w$ correctly if we plug in a number $w = A \in \mathbb{C}^+$. Representation (2.1) is useful here because it shows that $\log M(z)$ is holomorphic on $z \in \mathbb{C}^+$ and $\operatorname{Im} \log M(z) > 0$ there. Moreover, there is a similar formula for $i\pi - \log A$, which will show that $\operatorname{Im} \log M(z) < \pi$.

As anticipated, we now define the *Krein function* $\xi(t)$ as

$$\xi(t) = \frac{1}{\pi} \lim_{y \to 0+} \operatorname{Im} \log M(t+iy).$$

The limit will exist for almost all $t \in \mathbb{R}$. Of course, M has the same property, and if $M(t) = \lim M(t+iy)$ does exist, then also $\xi(t) = (1/\pi) \operatorname{Im} \log M(t)$ (though we cannot use (2.1) to compute the logarithm if $M(t)$ has real spectrum). Recall here that $\det M = -1$, so we still have $\sigma(M(t)) \subseteq \Omega$.

The above discussion shows that $0 \le \xi(t) \le 1$. Moreover, $\xi^t = \xi$ because M and thus also $\log M$ have this property.

We can deduce the additional properties of ξ listed in Proposition 1.1 most conveniently from the following elementary description of the matrix logarithm.

Lemma 2.1. *Suppose that $\sigma(A) \subseteq \Omega$. Then $B = \log A$ is the unique matrix satisfying $e^B = A$, $\sigma(B) \subseteq \{z : -\pi/2 < \operatorname{Im} z < 3\pi/2\}$.*

Sketch of proof. The above discussion has shown that $B = \log A$ has these properties. To prove that there is only one such B for a given A, notice that e^C is diagonalizable if and only if C is. This observation immediately gives us uniqueness of B when A is diagonalizable. It also implies that if A is not diagonalizable, then B must be of the form $B = \lambda + N$, $N^2 = 0$. In that case, since $\lambda = \lambda I$ and N commute, $e^B = e^\lambda(1+N)$, and again B is determined by A. □

3. Proof of Proposition 1.1

Part (a) is immediate from the formula

$$-1 = \det M(t) = \det e^{\log M(t)} = e^{\operatorname{tr} \log M(t)},$$

since $\operatorname{Im} \operatorname{tr} \log M(t) = \pi \operatorname{tr} \xi(t)$ and $0 \le \operatorname{tr} \xi(t) \le 2$.

To prove part (b), recall that (1.5) is equivalent to

$$\operatorname{Re} M(t) = 0; \tag{3.1}$$

compare [8, Proposition 7.8], [11, Lemma 8.1]. We can of course restrict our attention to those $t \in E$ for which $M(t)$ exists. Clearly, if $\xi(t) = 1/2$, then $M(t) = e^{\log M(t)} = e^{A(t)+i\pi/2} = ie^{A(t)}$ satisfies (3.1). Conversely, if (3.1) holds, then $M(t) = iB$ with $B > 0$ (recall again that $\det M(t) = -1$), so $B = e^A$ for some self-adjoint matrix A, and thus $\log M = A + i\pi/2$ by Lemma 2.1.

Similarly, in the situation of part (c), $\operatorname{Im} M(t) = 0$, so $M(t) = -\lambda P + (1/\lambda)(1 - P)$ for some $\lambda > 0$ and some projection P. Lemma 2.1 thus shows that $\log M(t) = (\log\lambda + i\pi)P - \log\lambda(1 - P)$, and in particular $\xi = P$ is the projection onto the negative eigenspace of $M(t)$.

4. Proof of Theorem 1.2

If $W \in \mathcal{R}(E)$, $\operatorname{tr} W = 0$, then $W(x)$ is real analytic [10, Theorem 4.1]. Moreover, $m_\pm(z)$ and $M(z)$ are holomorphic at $z = \infty$ [10, Lemma 1.2], and then [10, eqn. (5.6)] says that $m_+(z) = i - (q(0) + ip(0))/z + O(1/z^2)$, and here p, q are the entries of W, as in (1.4). While this is not explicitly done in [10], of course the same treatment applies to m_-, and it shows that similarly $m_-(z) = i + (q(0) - ip(0))/z + O(1/z^2)$. In terms of M, this means that

$$M(z) = i\left(1 - \frac{1}{z}W(0) + O(1/z^2)\right).$$

So, since the factor i commutes with everything and $\log(1 + A)$ can be computed in terms of its power series for $\|A\| < 1$, we have

$$\log M(z) = \frac{i\pi}{2} - \frac{1}{z}W(0) + O(1/z^2). \tag{4.1}$$

On the other hand, we can also obtain an asymptotic formula from (1.7). Write $\xi = \xi - 1/2 + 1/2$ and recall that $\xi = 1/2$ is the Krein function of $M(z) = i$ and $\xi = 1/2$ on E by Proposition 1.1(b). Hence

$$\begin{aligned}\log M(z) &= \frac{i\pi}{2} + \sum_{j=1}^{n}\int_{a_j}^{b_j}\frac{\xi(t) - 1/2}{t - z}\,dt\\ &= \frac{i\pi}{2} - \frac{1}{z}\sum_{j=1}^{n}\int_{a_j}^{b_j}(\xi(t) - 1/2)\,dt + O(1/z^2);\end{aligned}$$

notice that while (1.7) would normally deliver an extra constant matrix B on the right-hand side, we immediately see from the asymptotic expansions that this equals zero here. Comparison with (4.1) then shows that

$$W(0) = \sum_{j=1}^{n} \int_{a_j}^{b_j} (\xi(t) - 1/2)\, dt. \tag{4.2}$$

This only gives W at $x = 0$, but it actually suffices to discuss the claims of Theorem 1.2 for $x = x_0 = 0$ since $\mathcal{R}(E)$ and $\mathcal{R}_0(E)$ are invariant under shifts $W(x) \mapsto W(x+a)$.

Since $\|X - 1/2\| \le 1/2$ for any $X \ge 0$, $\operatorname{tr} X = 1$, the bound of Theorem 1.2 is immediate from (4.2) and Proposition 1.1(a).

To prove the final claims of Theorem 1.2, observe that $\|X - 1/2\| < 1/2$ unless $X = P$ is a projection. Moreover, the projections are the extreme points of the set of such matrices $X \ge 0$, $\operatorname{tr} X = 1$. Hence (4.2) also shows that $\|W(0)\| < (1/2)\sum(b_j - a_j)$ unless $\xi(t) \equiv P$ on $t \notin E$. We now finish the proof by showing that if ξ is of this form, so $\xi = 1/2$ on E, $\xi = P$ on E^c, then $M(z)$, defined via (1.7) with $A = 0$, is the M matrix of a $W \in \mathcal{R}_0(E)$.

Observe first of all that then M is holomorphic near $z = \infty$ and $M(\infty) = i$; compare also (4.3) below. This implies that $m_\pm$ have the same properties, and then we can conclude as in the proof of [10, Theorem 3.2] that M is the M matrix of a Dirac operator $L = L_W$. Recall in this context that $m_\pm(z)$ can be recovered from $M(z)$, for example as the eigenvectors of MJ, as follows:

$$M(z)J \begin{pmatrix} \pm m_\pm(z) \\ 1 \end{pmatrix} = \mp \begin{pmatrix} \pm m_\pm(z) \\ 1 \end{pmatrix}.$$

Also, we clearly have $W \in \mathcal{R}(E)$, by Proposition 1.1(b).

To show that $W \in \mathcal{R}_0(E)$, we again compute

$$\begin{aligned} \log M(z) &= \frac{i\pi}{2} + \sum_{j=1}^{n} \int_{a_j}^{b_j} \frac{\xi(t) - 1/2}{t - z}\, dt \\ &= \frac{i\pi}{2} + \sum_{j=1}^{n} \log \frac{b_j - z}{a_j - z} \left(P - \frac{1}{2} \right). \end{aligned} \tag{4.3}$$

This matrix is normal, with eigenvalues

$$\lambda_\pm(z) = \frac{i\pi}{2} \pm \frac{1}{2} \sum_{j=1}^{n} \log \frac{b_j - z}{a_j - z}, \tag{4.4}$$

and thus $M(z)$ will also be normal, with eigenvalues $e^{\lambda_\pm(z)}$. We also see from (4.3) that $\log M(z)$ and thus also $M(z)$ itself have holomorphic continuations through each gap (a_j, b_j). For $z = t \in (a_j, b_j)$, the corresponding logarithm from (4.4) has a negative argument, while all the other ones have positive arguments. Thus $\text{Im}\,\lambda_+(t) = \pi$, $\text{Im}\,\lambda_-(t) = 0$, and it follows that $\text{Im}\,M(t) = 0$. (The potential objection that was mentioned in the introduction does not apply here since $M(t)$ is normal, so $\text{Re}\,\log M(t)$, $\text{Im}\,\log M(t)$ do commute.) Hence $(a_j, b_j) \cap \sigma(L) = \emptyset$; in other words, $\sigma(L) \subseteq E$, and thus $L \in \mathcal{R}_0(E)$, as claimed.

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