Review notes

Introductory Fredholm theory and computation

**Issa Karambal · Veerle Ledoux ·
Simon J.A. Malham · Jitse Niesen**

20th November 2010

Abstract We provide an introduction to Fredholm theory and discuss using the Fredholm determinant to compute pure-point spectra.

Keywords Fredholm theory

Mathematics Subject Classification (2000) 65L15, 65L10

Issa Karambal · Simon J.A. Malham
Maxwell Institute for Mathematical Sciences
and School of Mathematical and Computer Sciences
Heriot-Watt University, Edinburgh EH14 4AS, UK
Tel.: +44-131-4513200
Fax: +44-131-4513249
E-mail: S.J.Malham@ma.hw.ac.uk

Veerle Ledoux
Vakgroep
Toegepaste Wiskunde en Informatica
Ghent University, Krijgslaan, 281-S9
B-9000 Gent, Belgium
E-mail: Veerle.Ledoux@ugent.be

Jitse Niesen
School of Mathematics
University of Leeds
Leeds, LS2 9JT, UK
E-mail: jitse@maths.leeds.ac.uk

1 Trace class and Hilbert–Schmidt operators

Before defining the Fredholm determinant we need to review some basic spectral and tensor algebra theory; to which this and the next sections are devoted. For this discussion we suppose that $\mathbb{H}$ is a $\mathbb{C}^n$-valued Hilbert space with the standard inner product $\langle\cdot,\cdot\rangle_{\mathbb{H}}$; linear in the second factor and conjugate linear in the first. Most of the results in this section are collated and extended from results in Simon [24–26] and Reed and Simon [27, 28]. We are interested in non-self adjoint trace class or Hilbert–Schmidt class linear operators $K \in \mathcal{L}(\mathbb{H})$.

1.1 Absolute value and polar decomposition

Definition 1 (Positive operator) An operator $K \in \mathcal{L}(\mathbb{H})$ is called *positive* if $\langle K\varphi,\varphi\rangle_{\mathbb{H}} \geqslant 0$ for all $\varphi \in \mathbb{H}$. We write $K \geqslant 0$ for such an operator and, for example, $K_1 \leqslant K_2$ if $K_2 - K_1 \geqslant 0$.

Note that every bounded positive operator on $\mathbb{H}$ is self-adjoint: $K^* = K$. For any $K \geqslant 0$ there is a unique operator $\sqrt{K}$ such that $K = (\sqrt{K})^2$. For any $K \in \mathcal{L}(\mathbb{H})$, note that $K^*K \geqslant 0$ since $\langle K^*K\varphi,\varphi\rangle_{\mathbb{H}} = \|K\varphi\|^2_{\mathbb{H}} \geqslant 0$. In particular, we define $|K| = \sqrt{K^*K}$. Lastly note that $\||K|\varphi\|^2_{\mathbb{H}} = \|K\varphi\|^2_{\mathbb{H}}$.

Theorem 1 (Polar decomposition) *There exists a unique operator U so that:*

1. $K = U\,|K|$*; this is the* polar decomposition *of K;*
2. $\|U\varphi\|_{\mathbb{H}} = \|\varphi\|_{\mathbb{H}}$ *for* $\varphi \in \overline{\mathrm{Ran}\,|K|} = (\ker K)^\perp$*;*
3. $\|U\varphi\|_{\mathbb{H}} = 0$ *for* $\varphi \in (\mathrm{Ran}\,|K|)^\perp = \ker K$*.*

Note that $|K| = U^*K$*.*

1.2 Compact operators and canonical expansion

We say that the bounded operator $K \in \mathcal{L}(\mathbb{H})$ has finite rank if $\mathrm{rank}(K) = \dim(\mathrm{Ran}K) < \infty$. A bounded operator K is call *compact* if and only if it is the norm limit of finite rank operators. More generally we have the following.

Definition 2 (Compact operators, Reed and Simon [27, p. 199]) Let $\mathbb{X}$ and $\mathbb{Y}$ be two Banach spaces. An operator $K \in \mathcal{L}(\mathbb{X},\mathbb{Y})$ is called *compact* (or completely continuous) if K takes bounded sets in $\mathbb{X}$ into precompact sets in $\mathbb{Y}$. Equivalently, K is compact if and only if for every bounded sequence $\{x_n\} \subset \mathbb{X}$, then $\{K\,x_n\}$ has a subsequence convergent in $\mathbb{Y}$.

Theorem 2 (Hilbert–Schmidt; see Reed and Simon [27, p. 203]) *Let K be a self-adjoint compact operator on $\mathbb{H}$. Then there is a complete orthonormal basis $\{\varphi_m\}$ for $\mathbb{H}$ so that $K\varphi_m = \lambda_m\varphi_m$.*

We use $\mathcal{J}_\infty = \mathcal{J}_\infty(\mathbb{H})$ to denote the family of compact operators.

Theorem 3 (Simon [26, p. 2]) *The family of compact operators $\mathcal{J}_\infty$ is a two-sided ideal closed under taking adjoints. In particular, $K \in \mathcal{J}_\infty$ if and only if $|K| \in \mathcal{J}_\infty$.*

Theorem 4 (Canonical expansion, Simon [26, p. 2]) *Suppose $K \in \mathcal{J}_\infty$, then K has a norm convergent expansion, for any $\phi \in \mathbb{H}$:*

$$K\,\phi = \sum_{m=1}^{N} \mu_m(K)\langle \varphi_m, \phi\rangle_{\mathbb{H}}\,\psi_m$$

where $N = N(K)$ is a finite non-negative integer or infinity, $\{\varphi_m\}_{m=1}^{N}$ and $\{\psi_m\}_{m=1}^{N}$ are orthonormal sets and the unique positive values $\mu_1(K) \geqslant \mu_2(K) \geqslant \ldots$ are known as the singular values *of K.*

1.3 Trace class and Hilbert–Schmidt ideals

Theorem 5 (Reed and Simon [27], p. 206-7) *Let $\mathbb{H}$ be a separable Hilbert space with orthonormal basis $\{\varphi_m\}_{m=1}^{\infty}$. Then for any positive operator $K \in \mathcal{L}(\mathbb{H})$, we define*

$$\operatorname{tr} K := \sum_{m=1}^{\infty} \langle \varphi_m, K\varphi_m\rangle_{\mathbb{H}}.$$

The number $\operatorname{tr} K$ is called the trace of K *and is independent of the orthonormal basis chosen. The trace has the following properties:*

1. $\operatorname{tr}(K_1 + K_2) = \operatorname{tr} K_1 + \operatorname{tr} K_2$;
2. $\operatorname{tr}(zK_1) = z \operatorname{tr} K_1$ *for all* $z \geqslant 0$;
3. $\operatorname{tr}(UK_1U^{-1}) = \operatorname{tr} K_1$ *for any unitary operator* U;
4. *If* $0 \leqslant K_1 \leqslant K_2$, *then* $\operatorname{tr} K_1 \leqslant \operatorname{tr} K_2$.

Definition 3 (Trace class) An operator $K \in \mathcal{L}(\mathbb{H})$ is called *trace class* if and only if $\operatorname{tr} K < \infty$. The family of all trace class operators is denoted $\mathcal{J}_1 = \mathcal{J}_1(\mathbb{H})$.

Theorem 6 (Reed and Simon [27], p. 207) *The family of trace class operators $\mathcal{J}_1(\mathbb{H})$ is a $*$-ideal in $\mathcal{L}(\mathbb{H})$, i.e.*

1. $\mathcal{J}_1$ *is a vector space;*
2. *If* $K_1 \in \mathcal{J}_1$ *and* $K_2 \in \mathcal{L}(\mathbb{H})$, *then* $K_1K_2 \in \mathcal{J}_1$ *and* $K_2K_1 \in \mathcal{J}_1$;
3. *If* $K \in \mathcal{J}_1$ *then* $K^* \in \mathcal{J}_1$.

We now collect some results together from Reed and Simon [27, p. 209].

Theorem 7 *We have the following results:*

1. *The space of operators $\mathcal{J}_1$ is a Banach space with norm $\|K\|_{\mathcal{J}_1} := \operatorname{tr}|K|$ and $\|K\| \leqslant \|K\|_{\mathcal{J}_1}$.*
2. *Every $K \in \mathcal{J}_1$ is compact. A compact operator K is in $\mathcal{J}_1$ if and only if $\sum \mu_m < \infty$ where $\{\mu_m\}_{m=1}^{\infty}$ are the singular values of K.*
3. *The finite rank operators are $\|\cdot\|_{\mathcal{J}_1}$-dense in $\mathcal{J}_1$.*

Definition 4 (Hilbert–Schmidt) An operator $K \in \mathcal{L}(\mathbb{H})$ is called *Hilbert–Schmidt* if and only if $\operatorname{tr} K^*K < \infty$. The family of Hilbert–Schmidt operators is denoted $\mathcal{J}_2 = \mathcal{J}_2(\mathbb{H})$.

Theorem 8 (Hilbert–Schmidt operators, Reed and Simon [27, p. 210]) *For the family of Hilbert–Schmidt operators, we have the following properties:*

1. *The family of operators* $\mathcal{J}_2$ *is a* $*$*-ideal;*
2. *If* $K_1, K_2 \in \mathcal{J}_2$*, then for any orthonormal basis* $\{\varphi_m\}$,

$$\sum_{m=1}^{\infty} \langle \varphi_m, K_1^* K_2\, \varphi_m \rangle_{\mathbb{H}}$$

   is absolutely summable, and its limit, denoted by $\langle K_1, K_2 \rangle_{\mathcal{J}_2}$*, is independent of the orthonormal basis chosen;*
3. $\mathcal{J}_2$ *with inner product* $\langle \cdot, \cdot \rangle_{\mathcal{J}_2}$ *is a Hilbert space;*
4. *If* $\|K\|_{\mathcal{J}_2} \coloneqq \sqrt{\langle K, K \rangle_{\mathcal{J}_2}} = (\operatorname{tr} K^* K)^{1/2}$*, then*

$$\|K\| \leqslant \|K\|_{\mathcal{J}_2} \leqslant \|K\|_{\mathcal{J}_1} \qquad \text{and} \qquad \|K\|_{\mathcal{J}_2} = \|K^*\|_{\mathcal{J}_2};$$

5. *Every* $K \in \mathcal{J}_2$ *is compact and a compact operator,* K*, is in* $\mathcal{J}_2$*, if and only if* $\sum \mu_m^2 < \infty$*, where the* μ_m *are the singular values of* K*;*
6. *The finite rank operators are* $\| \cdot \|_{\mathcal{J}_2}$*-dense in* $\mathcal{J}_2$*.*

Theorem 9 (Reed and Simon [27, p. 210]) *Let* $(\Omega, \mathrm{d}\nu)$ *be a measure space and* $\mathbb{H} = \mathbb{L}^2(\Omega, \mathrm{d}\nu)$ *The operator* $K \in \mathcal{L}(\mathbb{H})$ *is Hilbert–Schmidt if and only if there is a function* $G \in \mathbb{L}^2(\Omega \times \Omega, \mathrm{d}\nu \otimes \mathrm{d}\nu)$ *with*

$$(K\, U)(x) = \int G(x;\xi)\, U(\xi)\, \mathrm{d}\nu(\xi).$$

Further, we have that

$$\|K\|_{\mathcal{J}_2}^2 = \iint |G(x;\xi)|^2\, \mathrm{d}\nu(x)\, \mathrm{d}\nu(\xi).$$

Theorem 10 (Reed and Simon [27, p. 211]) *If* $\mathrm{K} \in \mathcal{J}_1$ *and* $\{\varphi_m\}_{m=1}^{\infty}$ *is any orthonormal basis, then* $\operatorname{tr} K$ *converges absolutely and the limit is independent of the choice of basis.*

Definition 5 (Trace, Reed and Simon [27, p. 211]) The map $\operatorname{tr}\colon \mathcal{J}_1 \to \mathbb{C}$ given by $\sum \langle \varphi_m, K \varphi_m \rangle_{\mathbb{H}}$ where $\{\varphi_m\}$ is any orthonormal basis is called the *trace*.

2 Multilinear algebra

2.1 Tensor product spaces

The *tensor product* of two vector spaces $\mathbb{V}$ and $\mathbb{W}$ over a field $\mathbb{K}$ is a vector space $\mathbb{V} \otimes \mathbb{W}$ equipped with a bilinear map

$$\mathbb{V} \times \mathbb{W} \to \mathbb{V} \otimes \mathbb{W}, \qquad v \times w \mapsto v \otimes w,$$

which is universal. The bilinear map is universal in the sense that for any bilinear map $\beta\colon \mathbb{V} \times \mathbb{W} \to \mathbb{U}$ to a vector space $\mathbb{U}$, there is a unique linear map from $\mathbb{V} \otimes \mathbb{W}$ to $\mathbb{U}$ that takes $v \otimes w$ to $\beta(v, w)$. This universality property determines the tensor product up to a canonical isomorphism.

Given a Hilbert space $\mathbb{H}$ with inner product $\langle\cdot,\cdot\rangle_{\mathbb{H}}$, we denote by $\mathbb{H}^{\otimes m}$ the tensor product $\mathbb{H}\otimes\cdots\otimes\mathbb{H}$ (m times). It is a vector space and if $\mathbb{H}=\operatorname{span}\{\varphi_k\}$ then

$$\mathbb{H}^{\otimes m}=\operatorname{span}\{\varphi_1\otimes\cdots\otimes\varphi_m\colon \varphi_1,\ldots,\varphi_m\in\mathbb{H}\}.$$

By convention $\mathbb{H}^{\otimes 0}$ is the ground field $\mathbb{K}$. We define an inner product on $\mathbb{H}^{\otimes m}$ by

$$\langle\varphi,\psi\rangle_{\mathbb{H}^{\otimes m}}:=\prod_{i=1}^{m}\langle\varphi_i,\psi_i\rangle_{\mathbb{H}}$$

for $\varphi=\varphi_1\otimes\cdots\otimes\varphi_m$ and $\psi=\psi_1\otimes\cdots\otimes\psi_m$. It is easy to show that if $\{\varphi_n\}_{n\in\mathbb{N}}$ is an orthonormal basis for $\mathbb{H}$ then $\{\varphi_{i_1}\otimes\cdots\otimes\varphi_{i_m}\}_{\{i_1,\ldots,i_m\}\in\mathbb{N}^m}$ is an orthonormal basis for $\mathbb{H}^{\otimes m}$ with respect to the inner product above. Given $K\in\mathcal{L}(\mathbb{H})$, there exists a natural linear operator $K^{\otimes m}\in\mathcal{L}(\mathbb{H}^{\otimes m})$ given by

$$K^{\otimes m}\colon \varphi_1\otimes\cdots\otimes\varphi_m\mapsto K\varphi_1\otimes\cdots\otimes K\varphi_m.$$

There are two natural subspaces of $\mathbb{H}^{\otimes m}$ namely, $\operatorname{Alt}^m\mathbb{H}$ or $\mathbb{H}^{\wedge m}$, the vector subspace of exterior (or alternating) powers, and $\operatorname{Sym}^m\mathbb{H}$, the vector subspace of symmetric powers. We briefly review these algebras here; we have mainly used Fulton and Harris [10, Appendix B] as a reference.

2.2 **Alternating algebra**

The exterior powers $\mathbb{H}^{\wedge m}$ of $\mathbb{H}$ come equipped with an alternating multilinear map

$$\mathbb{H}^{\times m}\to\mathbb{H}^{\wedge m},\qquad \varphi_1\times\cdots\times\varphi_m\mapsto\varphi_1\wedge\ldots\wedge\varphi_m,$$

that is universal. This means that for any alternating multilinear map $\beta\colon\mathbb{H}^{\times m}\to\mathbb{U}$ to a vector space $\mathbb{U}$, there is a unique linear map from $\mathbb{H}^{\times m}$ to $\mathbb{U}$ which takes $\varphi_1\wedge\ldots\wedge\varphi_m$ to $\beta(\varphi_1,\ldots,\varphi_m)$. A multilinear map is alternating if $\beta(\varphi_1,\ldots,\varphi_m)=0$ when any two arguments are equal. This is equivalent to the condition that $\beta(\varphi_1,\ldots,\varphi_m)$ changes sign whenever two arguments are interchanged. Hence we have, for any $\sigma\in\mathbb{S}_m$:

$$\beta(\varphi_{\sigma(1)},\ldots,\varphi_{\sigma(m)})=\operatorname{sgn}(\sigma)\,\beta(\varphi_1,\ldots,\varphi_m).$$

We can construct $\mathbb{H}^{\wedge m}$ as the quotient space of $\mathbb{H}^{\otimes m}$ by the subspace generated by all $\varphi_1\otimes\cdots\otimes\varphi_m$ with two of the components equal. We let

$$\pi\colon\mathbb{H}^{\otimes m}\to\mathbb{H}^{\wedge m},\qquad \pi\colon\varphi_1\otimes\cdots\otimes\varphi_m\mapsto\varphi_1\wedge\ldots\wedge\varphi_m,$$

denote the projection. If $\{\varphi_n\}$ is a basis for $\mathbb{H}$, then $\{\varphi_{i_1}\wedge\ldots\wedge\varphi_{i_m}\colon i_1<\cdots<i_m\}$, is a basis for $\mathbb{H}^{\wedge m}$. There is a natural embedding $\mathbb{H}^{\wedge m}\hookrightarrow\mathbb{H}^{\otimes m}$ defined by

$$\varphi_1\wedge\ldots\wedge\varphi_m\mapsto\frac{1}{\sqrt{m!}}\sum_{\sigma\in\mathbb{S}_m}\operatorname{sgn}(\sigma)\,\varphi_{\sigma(1)}\otimes\cdots\otimes\varphi_{\sigma(m)}.$$

The image of this embedding is the space of anti-invariants of the right action of $\mathbb{S}_m$ on $\mathbb{H}^{\otimes m}$.

Proposition 1 *The inner product in $\mathbb{H}^{\wedge m}$ generates a determinant:*

$$\langle\varphi_1\wedge\ldots\wedge\varphi_m,\psi_1\wedge\ldots\wedge\psi_m\rangle_{\mathbb{H}^{\otimes m}}=\det\bigl[\langle\varphi_i,\psi_j\rangle_{\mathbb{H}}\bigr].$$

Proof By direct computation, utilizing the natural embedding into $\mathbb{H}^{\otimes m}$ and the bilinearity properties of the inner product, we have

$$\begin{aligned}
&\langle \varphi_1 \wedge \ldots \wedge \varphi_m, \psi_1 \wedge \ldots \wedge \psi_m \rangle_{\mathbb{H}^{\otimes m}} \\
&\quad = \frac{1}{m!} \sum_{\sigma,\pi \in \mathbb{S}_m} \operatorname{sgn}(\sigma) \operatorname{sgn}(\pi) \left\langle \varphi_{\sigma(1)} \otimes \ldots \otimes \varphi_{\sigma(m)}, \psi_{\pi(1)} \otimes \ldots \otimes \psi_{\pi(m)} \right\rangle_{\mathbb{H}^{\otimes m}} \\
&\quad = \frac{1}{m!} \sum_{\sigma,\pi \in \mathbb{S}_m} \operatorname{sgn}(\sigma) \operatorname{sgn}(\pi) \prod_{i=1}^{m} \langle \varphi_{\sigma(i)}, \psi_{\pi(i)} \rangle_{\mathbb{H}} \\
&\quad = \frac{1}{m!} \sum_{\sigma \in \mathbb{S}_m} \operatorname{sgn}(\sigma) \det\left[\langle \varphi_{\sigma(i)}, \psi_j \rangle_{\mathbb{H}}\right] \\
&\quad = \det\left[\langle \varphi_i, \psi_j \rangle_{\mathbb{H}}\right].
\end{aligned}$$

□

Further note that $K^{\otimes m}$ leaves the subspace $\mathbb{H}^{\wedge m}$ of $\mathbb{H}^{\otimes m}$ invariant. We define $K^{\wedge m}$ to be the restriction of $K^{\otimes m}$ to $\mathbb{H}^{\wedge m}$.

2.3 Symmetric algebra

The symmetic powers $\operatorname{Sym}^m \mathbb{H}$ of $\mathbb{H}$ comes with a universal symmetric multilinear map

$$\mathbb{H}^{\times m} \to \operatorname{Sym}^m \mathbb{H}, \qquad \varphi_1 \times \cdots \times \varphi_m \mapsto \varphi_1 \cdot \ldots \cdot \varphi_m.$$

A multilinear map $\beta \colon \mathbb{H}^{\times m} \to \mathbb{U}$ is symmetric if it is unchanged when any two arguments are interchanged. Hence we have, for any $\sigma \in \mathbb{S}_m$:

$$\beta(\varphi_{\sigma(1)}, \ldots, \varphi_{\sigma(m)}) = \beta(\varphi_1, \ldots, \varphi_m).$$

We can construct $\operatorname{Sym}^m \mathbb{H}$ as the quotient space of $\mathbb{H}^{\otimes m}$ by the subspace generated by all $\varphi_1 \otimes \cdots \otimes \varphi_m - \varphi_{\sigma(1)} \otimes \cdots \otimes \varphi_{\sigma(m)}$, or by those in which σ permutes two successive factors. We let

$$\pi \colon \mathbb{H}^{\otimes m} \to \operatorname{Sym}^m \mathbb{H}, \qquad \pi \colon \varphi_1 \otimes \cdots \otimes \varphi_m \mapsto \varphi_1 \cdot \ldots \cdot \varphi_m,$$

denote the projection. If $\{\varphi_n\}$ is a basis for $\mathbb{H}$, then $\{\varphi_{i_1} \cdot \ldots \cdot \varphi_{i_m} : i_1 \leqslant \cdots \leqslant i_m\}$, is a basis for $\operatorname{Sym}^m \mathbb{H}$. There is a natural embedding $\operatorname{Sym}^m \mathbb{H} \hookrightarrow \mathbb{H}^{\otimes m}$ defined by

$$\varphi_1 \cdot \ldots \cdot \varphi_m \mapsto \frac{1}{\sqrt{m!}} \sum_{\sigma \in \mathbb{S}_m} \varphi_{\sigma(1)} \otimes \cdots \otimes \varphi_{\sigma(m)}.$$

For more details on *symmetric functions* see Macdonald [20].

2.4 **Hodge duality**

Let $\mathbb{H}^{\wedge m}$ denote the m-fold exterior product of the vector space $\mathbb{H}$, with inner product as given in Proposition 1 above. If $\varphi_1, \ldots, \varphi_N$ denote an orthonormal basis of $\mathbb{H}$, then as we have already seen,

$$\big\{\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m} : 1 \leqslant i_1 < \cdots < i_m \leqslant N\big\}$$

constitutes an orthonormal basis of $\mathbb{H}^{\wedge m}$. We define the *Hodge linear star operator* $\star\colon \mathbb{H}^{\wedge m} \to \mathbb{H}^{\wedge(N-m)}$ by

$$\star\colon \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m} \mapsto \varphi_{j_1} \wedge \ldots \wedge \varphi_{j_{N-m}}$$

where $0 \leqslant m \leqslant N$, and $j_1, \ldots, j_{N-m}$ are selected so that $\varphi_{i_1}, \ldots, \varphi_{i_m}, \varphi_{j_1}, \ldots, \varphi_{j_{N-m}}$ constitute a basis for $\mathbb{H}$; see for example Jost [18, pp. 87–9]. Note in particular we have

$$\begin{aligned} &\star\colon 1 \mapsto \varphi_1 \wedge \ldots \wedge \varphi_N, \\ &\star\colon \varphi_1 \wedge \ldots \wedge \varphi_N \mapsto 1. \end{aligned}$$

Further the following properties naturally follow: $\star\star = (-1)^{m(N-m)}\colon \mathbb{H}^{\wedge m} \to \mathbb{H}^{\wedge m}$; and $\star(K\psi_1 \wedge \ldots \wedge K\psi_m) = \det(K)\star(\psi_1 \wedge \ldots \wedge \psi_m)$ for any $\psi_1, \ldots, \psi_m \in \mathbb{H}$ and $N \times N$ matrix K. The following result can also be found in Jost [18, p. 88].

Lemma 1 *For any $\phi, \psi \in \mathbb{H}^{\wedge m}$ we have*

$$\langle \phi, \psi \rangle_{\mathbb{H}^{\wedge m}} = \star(\phi \wedge \star\psi) = \star(\psi \wedge \star\phi).$$

Remark 1 Note that we have $(\phi \wedge \star\psi) = \det([\phi]\ [\star\psi])$ where, if $\phi = \phi_1 \wedge \ldots \wedge \phi_m$, then $[\phi]$ denotes the matrix whose columns are $\phi_1, \ldots, \phi_m$. This latter result for the Evans function determinant was espoused by Bridges and Derks [5].

3 **Fredholm determinant for trace class operators**

3.1 **Motivation and definition**

Before we define the Fredholm determinant properly let us motivate our definition; see Reed and Simon [28, pp. 322-3] for more details. Suppose $K \in \mathcal{J}_1$ and also suppose $\mathbb{H}$ is finite dimensional, i.e. $\dim(\mathbb{H}) = N < \infty$. Let $\lambda_1, \ldots, \lambda_N$ be the eigenvalues for K and suppose $\varphi_1, \ldots, \varphi_N$ are a Schur basis (orthogonal eigenbasis) for $\mathbb{H}$. Then we see that

$$\det(\mathrm{id} + K) = \prod_{i=1}^{N}(1 + \lambda_i) = \big\langle \varphi_1 \wedge \ldots \wedge \varphi_N, (\mathrm{id} + K)\varphi_1 \wedge \ldots \wedge (\mathrm{id} + K)\varphi_N \big\rangle_{\mathbb{H}^{\wedge N}}.$$

We also see that for any $m \leqslant N$:

$$\begin{aligned} \mathrm{tr}\left(K^{\wedge m}\right) &= \sum_{i_1 < \cdots < i_m} \big\langle \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m}, (K^{\wedge m})(\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m}) \big\rangle_{\mathbb{H}^{\wedge m}} \\ &= \sum_{i_1 < \cdots < i_m} \langle \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_m}, K\varphi_{i_1} \wedge \ldots \wedge K\varphi_{i_m} \rangle_{\mathbb{H}^{\wedge m}} \\ &= \sum_{i_1 < \cdots < i_m} \lambda_{i_1} \cdots \lambda_{i_m}, \end{aligned}$$

where $i_1, \ldots, i_m \in \{1, \ldots, N\}$. Hence we observe that

$$\det(\mathrm{id} + K) = \sum_{m=0}^{N} \mathrm{tr}\left(K^{\wedge m}\right).$$

When $\mathbb{H}$ is an arbitrary separable Hilbert space (i.e. possibly infinite dimensional) we define $\det(\mathrm{id} + K)$ precisely in this way.

Definition 6 (Fredholm determinant, Grothendiek [14]) Let $K \in \mathcal{J}_1$, then $\det(\mathrm{id}+K)$ is defined by

$$\det(\mathrm{id} + K) := \sum_{m=0}^{\infty} \mathrm{tr}\left(K^{\wedge m}\right).$$

3.2 **Equivalent definitions**

Note that if $K \in \mathcal{J}_1(\mathbb{H})$ then $K^{\wedge m} \in \mathcal{J}_1(\mathbb{H}^{\wedge m})$ for all m. There are several equivalent definitions for $\det(\mathrm{id} + K)$ for $K \in \mathcal{J}_1$. For example for any $z \in \mathbb{C}$ we have

$$\det(\mathrm{id} + zK) = \prod_{m=1}^{N(K)} \big(1 + z\lambda_m(K)\big)$$

or

$$\det(\mathrm{id} + zK) = \exp\big(\mathrm{tr}\,\log(\mathrm{id} + zK)\big).$$

The latter definition is only determined modulo $2\pi i$ and it leads to the small z expansion known as Plemelj's formula:

$$\det(\mathrm{id} + zK) = \exp\Big(\sum (-1)^{m-1} z^m \,\mathrm{tr}\big(K^m\big)/m\Big),$$

which converges if $\mathrm{tr}\,|K| < 1$. The equivalence of these three definitions is established through Lidskii's theorem:

$$\mathrm{tr}\, K = \sum_{m=1}^{N(K)} \lambda_m(K).$$

There are two important properties of the determinant so defined. First the multiplication formula

$$\det(\mathrm{id} + K_1 + K_2 + K_1K_2) = \det(\mathrm{id} + K_1) \cdot \det(\mathrm{id} + K_2)$$

holds for all $K_1, K_2 \in \mathcal{J}_1$. Second, the characterization of invertibility: $\det(\mathrm{id}+K) \neq 0$ if and only if $(\mathrm{id} + K)^{-1}$ exists.

Remark 2 Note also that in the context of the exterior algebra of trace class operators, we can also think of the Fredholm determinant as

$$\det(\mathrm{id} + K) := \mathrm{tr}\left((\mathrm{id} - K)^{\wedge(-1)}\right).$$

Further we can also comfortably make equivalent statements in terms of the convolution algebra of the Green's kernels G.

3.3 **Fredholm determinant series expansion**

Here we suppose $\mathbb{H} = \mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$, the usual Hilbert space of Lebesgue square-integrable $\mathbb{C}^n$-valued functions on $\mathbb{R}$; the ground field $\mathbb{K} = \mathbb{R}$.

Proposition 2 *If $K \in \mathcal{J}_1$ so that $\operatorname{tr} K \coloneqq \sum \langle \varphi_m, K\varphi_m\rangle_{\mathbb{H}} < \infty$ for any basis $\{\varphi_m\}_{m=1}^{\infty}$, and the Green's integral kernel G (associated with K) is* continuous *on $\mathbb{R}^2$, then*

$$\operatorname{tr} K = \int_{\mathbb{R}} \operatorname{tr} G(x;x)\,\mathrm{d}x.$$

Remark 3 A proof for $n = 1$ is given in Simon [26, p. 35], and for $n \geqslant 1$ in Gohberg, Goldberg and Krupnik [13]. We essentially follow the latter.

Proof Let $\{\varphi_m\}_{m\geqslant 1}$ be an orthonormal basis for $\mathbb{H}$. Then the integral kernal $G = G(x;\xi)$ can be expanded columnwise in this basis:

$$G(x;\xi) = \sum_{m\geqslant 1} \varphi_m(x) G_m(\xi),$$

where $\varphi_m(x) \in \mathbb{C}^{n\times 1}$ and the coefficients $G_m(\xi) \in \mathbb{C}^{1\times n}$. Then explicitly computing the trace we get

$$\begin{aligned}
\operatorname{tr} K &= \sum_{\ell\geqslant 1} \langle \varphi_\ell, K\varphi_\ell\rangle_{\mathbb{H}} \\
&= \sum_{\ell,m\geqslant 1} \int_{\mathbb{R}^2} \big(\varphi_\ell(x)\big)^* \varphi_m(x) G_m(\xi)\varphi_\ell(\xi)\,\mathrm{d}\xi\,\mathrm{d}x \\
&= \sum_{\ell,m\geqslant 1} \int_{\mathbb{R}} \langle \varphi_\ell, \varphi_m\rangle_{\mathbb{H}} G_m(\xi)\varphi_\ell(\xi)\,\mathrm{d}\xi \\
&= \int_{\mathbb{R}} \sum_{m\geqslant 1} G_m(\xi)\varphi_m(\xi)\,\mathrm{d}\xi \\
&= \int_{\mathbb{R}} \operatorname{tr} G(\xi;\xi)\,\mathrm{d}\xi.
\end{aligned}$$

□

Lemma 2 *The following two useful identities hold:*

1. $G_m(\xi) = \langle \varphi_m, G(\cdot;\xi)\rangle_{\mathbb{H}}$;
2. $\langle \varphi_m, K\varphi_\ell\rangle_{\mathbb{H}} = \langle G_m^*, \varphi_\ell\rangle_{\mathbb{H}}$

Proof By direct computation we have that

$$\begin{aligned}
\langle \varphi_m, G(\cdot;\xi)\rangle_{\mathbb{H}} &= \sum_{\ell\geqslant 1} \int_{\mathbb{R}} \big(\varphi_m(x)\big)^* \varphi_\ell(x) G_\ell(\xi)\,\mathrm{d}x \\
&= \sum_{\ell\geqslant 1} \int_{\mathbb{R}} \big(\varphi_m(x)\big)^* \varphi_\ell(x)\,\mathrm{d}x\, G_\ell(\xi) \\
&= G_m(\xi),
\end{aligned}$$

and

$$\begin{aligned}\langle \varphi_m, K\varphi_\ell\rangle_{\mathbb{H}} &= \int_{\mathbb{R}^2} \big(\varphi_m(x)\big)^* G(x;\xi)\varphi_\ell(\xi)\,\mathrm{d}\xi\,\mathrm{d}x \\ &= \sum_{r\geqslant 1}\int_{\mathbb{R}^2} \big(\varphi_m(x)\big)^* \varphi_r(x) G_r(\xi)\varphi_\ell(\xi)\,\mathrm{d}\xi\,\mathrm{d}x \\ &= \sum_{r\geqslant 1}\int_{\mathbb{R}} \langle\varphi_m,\varphi_r\rangle_{\mathbb{H}} G_r(\xi)\varphi_\ell(\xi)\,\mathrm{d}\xi \\ &= \int_{\mathbb{R}} G_m(\xi)\varphi_\ell(\xi)\,\mathrm{d}\xi \\ &= \langle G_m^*, \varphi_\ell\rangle_{\mathbb{H}}.\end{aligned}$$

□

Proposition 3 (Fredholm series expansion) *If $K \in \mathcal{J}_1(\mathbb{H})$ and its associated Green's kernel G is continuous, then we have that*

$$\det(\mathrm{id}+K) \coloneqq \sum_{m=0}^{\infty} \mathrm{tr}\,\big(K^{\wedge m}\big),$$

where explicitly

$$\mathrm{tr}\,\big(K^{\wedge m}\big) = \frac{1}{m!}\sum_{\ell_1,\ldots,\ell_m=1}^{n}\int_{\mathbb{R}^m} \det\big[G_{\ell_i,\ell_j}(\xi_i,\xi_j)\big]_{i,j=1,\ldots,m}\,\mathrm{d}\xi_1\ldots\mathrm{d}\xi_m.$$

Remark 4 This is Fredholm's original formula and this result essentially establishes the equivalence of this with Grothendiek's form for $\det(\mathrm{id}+K)$ for *trace class operators with continuous integral kernels*. For more details, see Gohberg, Goldberg and Krupnik [13].

Proof By direct computation, we have that

$$\begin{aligned}\mathrm{tr}\,\big(\mathrm{K}^{\wedge m}\big) &= \sum_{i_1<\ldots<i_m} \det\big[\langle\varphi_{i_p}, K\varphi_{i_q}\rangle_{\mathbb{H}}\big]_{p,q\in\{1,\ldots,m\}} \\ &= \frac{1}{m!}\sum_{i_1,\ldots,i_m} \det\big[\langle\varphi_{i_p}, K\varphi_{i_q}\rangle_{\mathbb{H}}\big] \\ &= \frac{1}{m!}\sum_{i_1,\ldots,i_m} \det\big[\langle G_{i_p}^*, \varphi_{i_q}\rangle_{\mathbb{H}}\big] \\ &= \frac{1}{m!}\sum_{i_1,\ldots,i_m}\sum_{\sigma\in\mathbb{S}_m} \mathrm{sgn}(\sigma)\langle G_{\sigma(i_1)}^*, \varphi_{i_1}\rangle_{\mathbb{H}}\cdots\langle G_{\sigma(i_m)}^*, \varphi_{i_m}\rangle_{\mathbb{H}}.\end{aligned}$$

Explicitly writing out the product shown we get (superscripts indicate components)

$$\begin{aligned}&\langle G_{\sigma(i_1)}^*, \varphi_{i_1}\rangle_{\mathbb{H}}\cdots\langle G_{\sigma(i_m)}^*, \varphi_{i_m}\rangle_{\mathbb{H}} \\ &= \int_{\mathbb{R}^m} G_{\sigma(i_1)}(\xi_1)\varphi_{i_1}(\xi_1)\cdots G_{\sigma(i_m)}(\xi_m)\varphi_{i_m}(\xi_m)\,\mathrm{d}\xi_1\ldots\mathrm{d}\xi_m \\ &= \sum_{\ell_1,\ldots,\ell_m}\int_{\mathbb{R}^m} G_{\sigma(i_1)}^{\ell_1}(\xi_1)\varphi_{i_1}^{\ell_1}(\xi_1)\cdots G_{\sigma(i_m)}^{\ell_m}(\xi_m)\varphi_{i_m}^{\ell_m}(\xi_m)\,\mathrm{d}\xi_1\ldots\mathrm{d}\xi_m \\ &= \sum_{\ell_1,\ldots,\ell_m}\int_{\mathbb{R}^m} G_{i_1}^{\sigma^{-1}(\ell_1)}(\xi_{\sigma^{-1}(1)})\varphi_{i_1}^{\ell_1}(\xi_1)\cdots G_{i_m}^{\sigma^{-1}(\ell_m)}(\xi_{\sigma^{-1}(m)})\varphi_{i_m}^{\ell_m}(\xi_m)\,\mathrm{d}\xi_1\ldots\mathrm{d}\xi_m\end{aligned}$$

where we have used that all the terms in the product in the integrand are scalar and the relabelling symmetry for the integration variables. Note componentwise we have

$$\begin{aligned}\sum_{\sigma\in\mathbb{S}_m}\operatorname{sgn}(\sigma)\sum_{i_1,\ldots,i_m} & G_{i_1}^{\sigma^{-1}(\ell_1)}(\xi_{\sigma^{-1}(1)})\varphi_{i_1}^{\ell_1}(\xi_1)\cdots G_{i_m}^{\sigma^{-1}(\ell_m)}(\xi_{\sigma^{-1}(m)})\varphi_{i_m}^{\ell_m}(\xi_m)\\ &= \sum_{\sigma\in\mathbb{S}_m}\operatorname{sgn}(\sigma)G^{\ell_{\sigma^{-1}(1)},\ell_1}(\xi_{\sigma^{-1}(1)},\xi_1)\cdots G^{\ell_{\sigma^{-1}(m)},\ell_m}(\xi_{\sigma^{-1}(m)},\xi_m)\\ &= \det\big[G^{\ell_i,\ell_j}(\xi_i,\xi_j)\big]_{i,j\in\{1,\ldots,m\}}.\end{aligned}$$

Substituting these last few identities back into the expression above for $\operatorname{tr}\left(\mathrm{K}^{\wedge m}\right)$, and replacing superscripts for components by subscripts, gives the result. □

4 Determinant for Hilbert–Schmidt operators

Hilbert [17] showed how it was possible to extend Fredholm's theory to a wider class of operators than trace class, in particular to what are now known as Hilbert–Schmidt operators. In particular Hilbert developed a determinant series expansion much like the Fredholm determinant series expansion valid for Hilbert–Schmidt operators, where all the Green's kernel terms evaluated at the diagonal '$G(x,x)$' are set to zero. When the operator K is of trace class so that $\operatorname{tr}|K|<\infty$ then Hilbert's determinant '$\det_2$' and Fredholm's determinant, say '$\det_1$' from the last section, are related by

$$\det_2(\mathrm{id}+K)=\det_1(\mathrm{id}+K)\cdot\exp(-\operatorname{tr}K).$$

Let us begin the exposition in this section by establishing some properties of Hilbert–Schmidt operators; here we mainly follow Bornemann [3]. Note that the product of two Hilbert–Schmidt operators is of trace class:

$$\|K_1K_2\|_{\mathcal{J}_1}\leqslant\|K_1\|_{\mathcal{J}_2}\,\|K_2\|_{\mathcal{J}_2}.$$

For a Hilbert–Schmidt operator $K\in\mathcal{J}_2(\mathbb{H})$ we have that

$$\operatorname{tr}K^2=\sum_{m=1}^{N(K)}\big(\lambda_m(K)\big)^2<\infty\qquad\text{and}\qquad|\operatorname{tr}K^2|\leqslant\sum_{m=1}^{N(K)}\big|\lambda_m(K)\big|^2\leqslant\|K\|_{\mathcal{J}_2}^2.$$

For a general Hilbert–Schmidt operator we only know the convergence of $\sum\big(\lambda_m(K)\big)^2$ but not of $\sum\lambda_m(K)$. Hence the Fredholm determinants defined in the last section do not converge in general. For $K\in\mathcal{J}_2(\mathbb{H})$ we define

$$\det_2(\mathrm{id}+z\,K)\coloneqq\prod_{m=1}^{N(K)}\big(1+z\,\lambda_m(K)\big)\,\exp(-z\lambda_m(K))$$

which possesses zeros at $z_m=-1/\lambda_m(K)$, counting multiplicity. Plemelj's formula now has the form

$$\det_2(\mathrm{id}+z\,K)=\exp\bigg(-\sum_{m=2}^{\infty}\frac{(z)^m}{m}\operatorname{tr}K^m\bigg),$$

for $|z| < 1/|\lambda_1(K)|$. Note that K^2, K^3, ... are trace class if $K \in \mathcal{J}_2$. Further, if $K \in \mathcal{J}_2(\mathbb{H})$ then $(\mathrm{id} + z\,K)\exp(-z\,K) - \mathrm{id} \in \mathcal{J}_1(\mathbb{H})$ and we have

$$\det{}_2(\mathrm{id} + z\,K) = \det{}_1\Big(\mathrm{id} + \big((\mathrm{id} + z\,K)\exp(-z\,K) - \mathrm{id}\big)\Big).$$

If $\mathbb{H} = \mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$ then Hilbert–Schmidt operators are exactly given by integral operators with a square integrable kernel. In other words there is one-to-one correspondence between $K \in \mathcal{J}_2(\mathbb{H})$ and $G \in \mathbb{L}^2(\mathbb{R}^2;\mathbb{C}^{n\times n})$ given by

$$(K\,U)(x) = \int_{\mathbb{R}} G(x;\xi)\,U(\xi)\,\mathrm{d}\xi.$$

Indeed we have $\|K\|_{\mathcal{J}_2} = \|G\|_{\mathbb{L}^2}$ so that $\mathcal{J}_2(\mathbb{H})$ and $\mathbb{L}^2(\mathbb{R}^2;\mathbb{C}^{n\times n})$ are isometrically isomorphic. Further we have the expansion (for the scalar case with $n = 1$) that $\det_2(\mathrm{id} + zK)$ is given by

$$\sum_{m=0}^{\infty} \frac{z^m}{m!} \int_{\mathbb{R}^m} \det \begin{pmatrix} 0 & G(x_1;x_2) & \cdots & G(x_1;x_m) \\ G(x_2;x_1) & 0 & \cdots & G(x_2;x_m) \\ \vdots & \vdots & \ddots & \vdots \\ G(x_m;x_1) & G(x_m;x_2) & \cdots & 0 \end{pmatrix} \mathrm{d}x_1 \ldots \mathrm{d}x_m$$

Proof See Simon [26, Theorem 9.4].

Remark 5 If $K \notin \mathcal{J}_1(\mathbb{H})$ then $\int G(x;x)\,\mathrm{d}x \neq \mathrm{tr}\,K$; because $\mathrm{tr}\,K$ is not well defined.

Remark 6 Some more details in Fredholm Theory can be found in Chapter 5 of Barry Simon's *Trace ideals and their applications* book [26]. In particular the following useful between the Fredholm determinant of K, the resolvent operator $(\mathrm{id} + K)^{-1}$ and the derivative $\mathrm{D}f$ of the map $f\colon K \mapsto \det(\mathrm{id} + K)$ is proved:

$$\mathrm{D}f(K) = (\mathrm{id} + K)^{-1}\,\det(\mathrm{id} + K).$$

This result for example, implies that

$$(\mathrm{id} + zK)^{-1} = 1 + \frac{z\mathrm{D}f(zK)}{\det(\mathrm{id} + zK)}.$$

Further, for any $K \in \mathcal{J}_1$, we have the Plemelj–Smithies formulae, $\det(\mathrm{id} + zK) = \sum_{m\geqslant 0} z^m \alpha_m K/m!$ and $\mathrm{D}(zK) = \sum_{m\geqslant 0} z^{m+1}\beta_m K/m!$, where

$$\alpha_m(K) = \det \begin{pmatrix} \mathrm{tr}K & m-1 & \cdots & 0 \\ \mathrm{tr}K^2 & \mathrm{tr}K & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{tr}K^m & \mathrm{tr}K^{m-1} & \cdots & \mathrm{tr}K \end{pmatrix}$$

and

$$\beta_m(K) = \det \begin{pmatrix} K & m & 0 & \cdots \\ K^2 & \mathrm{tr}K & m-1 & \cdots \\ \vdots & \vdots & \ddots & \vdots \\ K^{m+1} & \mathrm{tr}K^m & \cdots & \mathrm{tr}K^{m-1} \end{pmatrix}.$$

5 Fredholm determinant construction

How would we actually use Fredholm theory to solve the original eigenvalue problem

$$\mathcal{L}u = \lambda\, u \qquad \Leftrightarrow \qquad \mathcal{L}(\lambda)u = 0$$

for a given linear operator $\mathcal{L}$ or equivalently $\mathcal{L}(\lambda) \coloneqq \mathcal{L} - \lambda\,\mathrm{id}$? Throughout this section, we suppose $\mathbb{H} = \mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$ and λ is the *spectral parameter*. We could attempt to directly invert $\mathcal{L}(\lambda)$ but the usual strategy, as advocated by Simon [26], is as follows. Suppose that we can decompose $\mathcal{L}(\lambda)$ as

$$\mathcal{L}(\lambda) = \mathcal{L}_0(\lambda) + \hat{\mathcal{L}}$$

where we suppose the linear operator $\hat{\mathcal{L}}$ contains the potential term and is such that $\hat{\mathcal{L}} \to 0$ as $x \to -\infty$ (this choice as opposed to $x \to +\infty$ is arbitrary for the moment). Then in some sense $\mathcal{L}_0(\lambda)$ is the operator associated with the base background state, i.e. for which their is no potential or it is zero (we will be more precise presently). Importantly $\mathcal{L}_0(\lambda)$ is a *constant coefficient differential operator* and we can write down an explicit analytical solution to the partial differential equations for the Green's kernel corresponding to $K_0(\lambda) = \mathcal{L}_0^{-1}(\lambda)$. Hence we rewrite the eigenvalue problem above as

$$\big(\mathcal{L}_0(\lambda) + \hat{\mathcal{L}}\big)\, u = 0 \qquad \Leftrightarrow \qquad \big(\mathrm{id} + K_0(\lambda) \circ \hat{\mathcal{L}}\big)\, u = 0.$$

The idea now would be to compute the [Fredholm] determinant

$$\det\big(\mathrm{id} + K_0(\lambda) \circ \hat{\mathcal{L}}\big).$$

Note that often $\hat{\mathcal{L}}$ is simply a bounded linear operator (though not always—when it is a lower order differential operator we can can integrate by parts). To compute this Fredholm determinant, one option is to compute the terms in the Fredholm determinant series up to a certain order, or for example to use Bornemann's numerical approach [3].

6 Green's integral kernels

6.1 Classical theory

We suppose now that $\mathbb{H}$ is the Hilbert space $\mathbb{L}^2(\Omega;\mathbb{C}^n)$ of $\mathbb{C}^n$-valued functions on the domain $\Omega \subseteq \mathbb{R}^d$. Let $\mathcal{L}$ denote a general linear differential operator from $\mathrm{dom}(\mathcal{L}) \subseteq \mathbb{H}$ to $\mathbb{H}$. If $\langle\,\cdot\,,\,\cdot\,\rangle_{\mathbb{H}}$ denotes the inner product, then we classically define the *adjoint operator* $\mathcal{L}^*$ through the relation

$$\langle \mathcal{L}^* u, v\rangle_{\mathbb{H}} = \langle u, \mathcal{L}v\rangle_{\mathbb{H}}$$

for all $u, v \in \mathbb{H}$ for which each side is meaningful. Let K be a Hilbert–Schmidt operator. We know from Theorem 9 above that there exists a function $G \in \mathbb{L}^2(\Omega \times \Omega;\mathbb{C}^{n\times n})$ such that

$$K \colon U \mapsto \int_\Omega G(\,\cdot\,;\xi)\, U(\xi)\,\mathrm{d}\xi.$$

We seek the integral operator K such that

$$\mathcal{L} \circ K = K \circ \mathcal{L} = \mathrm{id}$$

holds in $\mathcal{J}_2$, i.e. that K is the formal inverse operator of $\mathcal{L}$. Indeed, suppose the corresponding Green's kernel G (to K) satisfies the pair of partial differential equations

$$\mathcal{L}_x\, G(x;\xi) = \delta(x-\xi)\,\mathrm{id}_n,$$
$$\mathcal{L}^*_\xi\, G(x;\xi) = \delta(x-\xi)\,\mathrm{id}_n.$$

Then by direct computation and the properties of the Dirac delta function δ we see that

$$\big(\mathcal{L}\circ K\big)(U)(x) = \mathcal{L}_x \circ \int_\Omega G(x;\xi)\,U(\xi)\,\mathrm{d}\xi = \int_\Omega \delta(x-\xi)\,U(\xi)\,\mathrm{d}\xi = U(x),$$

and

$$\big(K\circ\mathcal{L}\big)(U)(x) = \int_\Omega G(x;\xi)\,\mathcal{L}_\xi U(\xi)\,\mathrm{d}\xi = \int_\Omega \big(\mathcal{L}^*_\xi G(x;\xi)\big)\,U(\xi)\,\mathrm{d}\xi = U(x),$$

which proves the result. Note that in particular, the Green's kernel corresponding to $K = \mathrm{id}$ is $G(x;\xi) = \delta(x-\xi)\,\mathrm{id}_n$.

In the rest of this section we consider the case of general linear operators on $\Omega = \mathbb{R}$ for which we can explicitly compute important results (the restriction to any finite or semi-infinite subdomain of $\mathbb{R}$ is straightforward).

6.2 **Green's function construction**

Consider the following nth order operator on $\mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$:

$$\mathrm{D}_A \colon U \mapsto \partial_x U - A\,U.$$

Indeed we see that $\mathrm{D}_A \colon \mathbb{H}^1(\mathbb{R};\mathbb{C}^n) \to \mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$, since $\mathrm{dom}(\mathrm{D}_A) \subseteq \mathbb{H}^1(\mathbb{R};\mathbb{C}^n)$. Here $A = A(x;\lambda) \in \mathbb{C}^{n\times n}$ depends on a (eigenvalue) parameter λ. Our first goal is to establish the existence of the inverse operator $\mathrm{K}_A \colon \mathbb{L}^2(\mathbb{R};\mathbb{C}^n) \to \mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$ of D_A. To this end we determine the vector subspaces of solutions $\ker(\mathrm{D}_A) \cap \mathbb{L}^2(\mathbb{R}_-;\mathbb{C}^n)$ and $\ker(\mathrm{D}_A) \cap \mathbb{L}^2(\mathbb{R}_+;\mathbb{C}^n)$. We assume there exists some $1 \leqslant k \leqslant n$ for which

$$\ker(\mathrm{D}_A) \cap \mathbb{L}^2(\mathbb{R}_-;\mathbb{C}^n) \subseteq \mathbb{L}^2\big(\mathbb{R}_-;\mathbb{V}(n,k)\big)$$

and

$$\ker(\mathrm{D}_A) \cap \mathbb{L}^2(\mathbb{R}_+;\mathbb{C}^n) \subseteq \mathbb{L}^2\big(\mathbb{R}_+;\mathbb{V}(n,n-k)\big).$$

Here $\mathbb{V}(n,k)$ respresents the *Stiefel manifold* of k-frames in $\mathbb{C}^n$, centred at the origin. Implicitly we are assuming that $n \geqslant 2$ (and hereafter).

The *adjoint operator* D^*_A and is defined as the operator $\mathrm{D}^*_A \colon \mathbb{H}^1\big(\mathbb{R};\mathbb{C}^n\big) \to \mathbb{L}^2\big(\mathbb{R};\mathbb{C}^n\big)$:

$$\mathrm{D}^*_A \colon Z \mapsto -\partial_x Z - A^*\,Z.$$

The *cokernel* of D_A is $\mathrm{coker}(\mathrm{D}_A) = \ker(\mathrm{D}^*_A)$. Note that the dimensions of $\ker(\mathrm{D}_A)$ and $\mathrm{coker}(\mathrm{D}_A)$ on $\mathbb{R}$ thus match, both are equal to k. Hence the *Fredholm index* given by

$$\dim\big(\ker(\mathrm{D}_A)\big) - \dim\big(\mathrm{coker}(\mathrm{D}_A)\big)$$

is thus zero under the assumptions above.

We establish here the existence of the inverse operator K_A of D_A. We assume that we can express $\mathrm{K}_A\colon \mathbb{L}^2(\mathbb{R};\mathbb{C}^n)\to\mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$ in the form

$$\mathrm{K}_A\colon U\mapsto \int_{\mathbb{R}} G(\,\cdot\,;\xi)\,U(\xi)\,\mathrm{d}\xi,$$

where $G\in\mathbb{L}^2(\mathbb{R}^2;\mathbb{C}^{n\times n})$ is a *Green's integral kernel* function.

Remark 7 (Important warning.) For any general nth order operator of the form D_A, the integral kernal $G=G(x;\xi)$ will not be continuous on $\mathbb{R}^2$. Indeed let Δ_- denote the simplex or half-plane below the forty-five degree line, $\xi<x$, and Δ_+ the simplex above it, $\xi>x$. Then G will be discontinuous exactly along the boundary denoting the border between Δ_- and Δ_+, and smooth elsewhere. However, suppose that we obtained D_A through prolongation. By this we mean that we defined additional variables so that we obtained a system of $2n$ first order linear operators D_A from a system of, say, n second order operators $\mathcal{L}$. Two important observations are crucial here. First that we could in principle invert the operator $\mathcal{L}$ directly to obtain K which will have an $n\times n$ matrix valued kernel G. The kernel G *will be trace class* and in particular continuous. This is because we have integrated the system of second order partial differential equations for G, as described above, twice. Indeed, an important strategy is to pursue this approach when applying Bornemann's numerical approach to computing the Fredholm determinant. Note further that if we invert the operator D_A, the corresponding $2n\times 2n$ Green's kernel should of course generate the same Fredholm determinant!

Following the classical theory above, suppose the Green's integral kernel $G\in\mathbb{L}^2(\mathbb{R}^2;\mathbb{C}^{n\times n})$ satisfies the partial differential equations:

$$\mathrm{D}_A G(x;\cdot)=\delta(x-\xi)\,\mathrm{id}_n \qquad\Leftrightarrow\qquad \partial_x G(x;\xi)-A(x)\,G(x;\xi)=\delta(x-\xi)\,\mathrm{id}_n$$

and

$$\mathrm{D}_A^* G(\cdot;\xi)=\delta(x-\xi)\,\mathrm{id}_n \qquad\Leftrightarrow\qquad -\partial_\xi G(x;\xi)-A^*(\xi)\,G(x;\xi)=\delta(x-\xi)\,\mathrm{id}_n.$$

Then the integral kernel G is the classical Green's kernel for K_A. Indeed K_A exists and we have $\mathrm{K}_A\circ\mathrm{D}_A=\mathrm{D}_A\circ\mathrm{K}_A=\mathrm{id}$.

We can in fact be much more explicit about the form of G. Indeed we can identify $\ker(\mathrm{D}_A)\cap\mathbb{L}^2(\mathbb{R}_-;\mathbb{C}^n)$ precisely—computing it either analytically or numerically as the solution of the homogeneous ordinary differential system generated by D_A. We label the solution manifold by $Y^-\in\mathbb{L}^2(\mathbb{R}_-;\mathbb{V}(n,k))$. Similarly, let $Y^+\in\mathbb{L}^2(\mathbb{R}_+;\mathbb{V}(n,n-k))$ be the solution manifold for $\ker(\mathrm{D}_A)\cap\mathbb{L}^2(\mathbb{R}_+;\mathbb{C}^n)$. Further, let Z^- and Z^+ be the solution manifolds, respectively, of $\ker(\mathrm{D}_A^*)\cap\mathbb{L}^2(\mathbb{R}_-;\mathbb{C}^n)$ and $\ker(\mathrm{D}_A^*)\cap\mathbb{L}^2(\mathbb{R}_+;\mathbb{C}^n)$.

Definition 7 (Green's integral kernel) We define the *Green's integral kernel* function G associated with K_A to be the map

$$G\colon \Delta_\pm\to\big\{\ker(\mathrm{D}_A)\cap\mathbb{L}^2(\mathbb{R}_\mp;\mathbb{C}^n)\big\}\times\big\{\ker(\mathrm{D}_A^*)\cap\mathbb{L}^2(\mathbb{R}_\pm;\mathbb{C}^n)\big\}\cong\mathbb{C}^{n\times n}$$

given by

$$G\colon (x;\xi)\mapsto\begin{cases} Y^-(x)\,\big(Z^+(\xi)\big)^*, & \xi>x,\\ -Y^+(x)\,\big(Z^-(\xi)\big)^*, & \xi<x.\end{cases}$$

An important property is that the functions $Y_j^{\pm}$ and $Z_i^{\pm}$ which lie in the kernels of D_A and D_A^*, respectively, satisfy the constraint

$$\frac{\mathrm{d}}{\mathrm{d}x}\langle Z_i^+, Y_j^-\rangle_{\mathbb{C}^n} = \frac{\mathrm{d}}{\mathrm{d}x}\langle Z_i^-, Y_j^+\rangle_{\mathbb{C}^n} = 0.$$

This follows by direct computation (and can be interpreted in terms of the definition of the adjoint operator D_A^*). We can in fact normalize $Y_j^{\pm}$ and $Z_i^{\pm}$ to obtain the following.

Lemma 3 *The kernels of* D_A *and* D_A^* *form orthonormal sets on* $\mathbb{R}$*, i.e. we have*

$$\langle Z_i^+, Y_j^-\rangle_{\mathbb{C}^n} = \langle Z_i^-, Y_j^+\rangle_{\mathbb{C}^n} = \delta_{ij},$$

where for Y_j^- *and* Z_i^-, $i,j \in \{1,\ldots,k\}$*, while for* Y_j^+ *and* Z_i^+, $i,j \in \{1,\ldots,n-k\}$.

Remark 8 The Green's integral kernel just defined satisfies the partial differential equations of the classical theory. The *compatability condition*—that there is a unit jump in the solution due to the delta function along $\xi = x$—is equivalent to the requirement that $Y^+(x)\big(Z^-(x)\big)^* + Y^-(x)\big(Z^+(x)\big)^* = \mathrm{id}_n$ for all $x \in \mathbb{R}$. It can also be expressed as the condition for all $x \in \mathbb{R}$: $\big(Y^-(x)\ Y^+(x)\big)\ \big(Z^+(x)\ Z^-(x)\big)^* = \mathrm{id}_n$. The integral operator K_A has the appropriate properties as an inverse of D_A if and only if the *compatability condition* is satisfied. There are several perspectives we can bring to this. Note that both matrices on the left are $n \times n$. Hence the compatability condition is equivalent to the requirement that $Z^+(x)$ and $Z^-(x)$ are generated by the inverse of $\big(Y^-(x)\ Y^+(x)\big)$. The inverse exists if and only if $\det\big(Y^-(x)\ Y^+(x)\big) \neq 0$. Note that $\det\big(Y^-(x)\ Y^+(x)\big)$ is the usual *Evans function*. Our original eigenvalue problem is generated by the operator $\mathrm{D}_A \coloneqq \partial_x - A$ on $\mathbb{L}^2(\mathbb{R};\mathbb{C}^n)$, where $A = A(x;\lambda) \in \mathbb{C}^{n\times n}$. Hence if $\det\big(Y^-(x)\,Y^+(x)\big) \neq 0$, then the inverse K_A exists, and any solution is trivial. Nontrivial solutions correspond to $\det\big(Y^-(x)\ Y^+(x)\big) = 0$.

Hence suppose we rewrite our spectral problem for $\mathcal{L}(\lambda)$ in the form

$$\big(\partial_x - A(x;\lambda)\big)Y = 0 \qquad \Leftrightarrow \qquad \mathrm{D}_{A(x;\lambda)}Y = 0.$$

We follow the strategy we outlined at the end of the last section, but for $\mathrm{D}_{A(x;\lambda)}$ instead of $\mathcal{L}(\lambda)$. The key is to decompose the coefficient matrix $A(x;\lambda)$ as follows:

$$A(x;\lambda) = A_0(\lambda) + A_1(x)$$

where $A_0(\lambda)$ is constant and $A_1 \to O$ as $x \to -\infty$. We form the corresponding nth order operator

$$\mathrm{D}_{A_0(\lambda)} \coloneqq \partial_x - A_0(\lambda).$$

Our original eigenvalue problem can now be expressed in the form

$$\mathrm{D}_{A_0(\lambda)}Y = A_1 Y \qquad \Leftrightarrow \qquad \big(\mathrm{id} - \mathrm{K}_{A_0(\lambda)} \circ A_1\big)Y = O,$$

where $\mathrm{K}_{A_0(\lambda)}$ is the integral operator that is the inverse of $\mathrm{D}_{A_0(\lambda)}$. We are thus now interested in computing the Fredholm determinant

$$\det{}_{\mathrm{F}}\Big(\mathrm{id} - \mathrm{K}_{A_0(\lambda)} \circ A_1\Big).$$

Acknowledgements We have unashamedly relied heavily on the classical books of Barry Simon [26] and Reed and Simon [27,28], whose exposition we can in no shape or form improve upon, but merely re-interpret in our own minds as we have done so here. We were inspired to learn more about Fredholm theory after reading the paper by Folkmar Bornemann [3]. His computational technique for computing spectra and our desire to understand it, sparked the need for us, to produce these notes.

References

1. J.C. Alexander, R. Gardner and C.K.R.T. Jones, *A topological invariant arising in the stability analysis of traveling waves*, J. Reine Angew. Math. 410 (1990), pp. 167–212.
2. F. Bergeron, *Algebraic combinatorics and co-invariant spaces*, CMS Treatises in Mathematics, Canadian Mathematical Society, 2009.
3. F. Bornemann, *On the numerical evaluation of Fredholm determinants*, Math. Comp. 79(270) (2010), pp. 871–915.
4. R. Bott and L.W. Tu, *Differential forms in Algebraic topology*, Graduate Texts in Mathematics 82, Springer 1982.
5. T.J. Bridges and G. Derks, *Hodge duality and the Evans function*, Physics Letters A 251 (1999), pp. 363–372.
6. C. Brouder, B. Fauser, A. Frabetti and R. Oeckl, *Quantum field theory and Hopf algebra cohomology*, Journal of Physucs A: Mathematical and General 37 (2004), pp. 5895–5927.
7. A. Connes and D. Kreimer, *Renormalization in quantum field theory and the Riemann–Hilbert problem I: The Hopf algebra structure of graphs and the main theorem*, Commun. Math. Phys. 210 (2000), pp. 249–273.
8. J. Deng and C. Jones, *Multi-dimensional Morse index theorems and a symplectic view of elliptic boundary value problems*, submitted to Transactions of the American Mathematical Society, 2009.
9. I. Fredholm, *Sur une classe d'équations fonctionnelles*, Acta. Math. 27 (1903), pp. 365–390.
10. W. Fulton and J. Harris, *Representation theory: A first course*, Graduate Texts in Mathematics 129, Springer, 2004.
11. W. Fulton and P. Pragacz, *Schubert varieties and degeneracy loci*, Lecture notes in mathematics 1689, Springer 1998.
12. K. Furutani, *Review: Fredholm–Lagrangian–Grassmannian and the Maslov index*, Journal of Geometry and Physics 51 (2004), pp. 269–331.
13. I. Gohberg, S. Goldberg, and N. Krupnik, *Traces and determinants of linear operators*, Birkhäuser, 2000.
14. A. Grothendiek, *La théorie de Fredholm*, Bull. Soc. Math. France 84 (1956), pp. 319–384.
15. N. Higson, *The residue index theorem of Connes and Miscovici*, Clay Mathematics Proceedings, American Mathematical Society, 2004.
16. N. Higson and J. Roe, *Lectures on operator K-theory and the Atiyah–Singer index theorem*, August 17, 2004.
17. D. Hilbert, *Grundzüge einer allgemeinen Theorie der linearen Integralgleichungen* (Erste Mitteilung), Nachr. Ges. Wiss. Göttingen (1904), pp. 49–91.
18. J. Jost, *Riemannian geometry and geometric analysis*, Universitext, Fifth Edition, Springer 1995.
19. G. Khimshiashvili, *Geometric aspects of Riemann–Hilbert problems*, Memoirs on Differential Equations and Mathematical Physics 27 (2002), pp. 1–114.
20. I.G. Macdonald, *Symmetric functions and Hall polynomials*, Clarendon Press, Oxford, 1979.
21. , C.D. Meyer, *Matrix analysis and applied linear algebra*, SIAM, 2000.
22. A. Pressley and G. Segal, *Loop groups*, Oxford Mathematical Monographs, Clarendon Press, Oxford, 1986.
23. M. Puschnigg, *Characters of Fredholm modules and a problem of Connes*, Geometric and Functional Analysis 18 (2008), pp. 583–635.
24. B. Simon, *Notes on infinite determinants of Hilbert space operators*, Advances in Mathematics 24 (1977), pp. 244–273.
25. B. Simon, *Resonances in one dimension and Fredholm determinants*, J. Funct. Anal. 178 (2000), pp. 396–420.
26. B. Simon, *Trace ideals and their applications*, Mathematical Surveys and Monographs, Volume 120, AMS, 2nd Ed. , 2005.
27. M. Reed and B. Simon, *Methods of modern mathematical physics I: Functional analysis*, Academic Press, 1980.
28. M. Reed and B. Simon, *Methods of modern mathematical physics IV: Analysis of operators*, Academic Press, 1978.
29. J. Robbin and D. Salamon: *The spectral flow and the Maslov index*, Bull. London Math. Soc. 27 (1995), pp. 1–33.
30. B. Sandstede, *Stability of travelling waves*, In Handbook of Dynamical Systems II, B. Fiedler, ed., Elsevier (2002), pp. 983–1055.