

UNIVERSITY OF POTSDAM

BACHELOR THESIS

Investigation of Functionals of the Eigenvalues of Unitary Matrices

Author:
Carina SEIDEL

Supervisor:
Dr. Thomas MACH

June 7, 2025



Abstract

The eigenvalues of large matrices are of interest for a large variety of use cases. Their calculation however grows increasingly complex with increasing matrix sizes. Therefore, we seek to simplify this process by approximating functionals over the spectrum of a matrix. This thesis is focussed on the spectral density or Denisty of States (DoS) among those.

Contents

1	Introduction	2
1.1	Unitary Matrices	2
1.2	Cayley Transform	3
1.3	Spectral Density	3

Introduction

To kick off this investigation we first need to look closer at unitary matrices and their properties. Then we will reiterate over the cayley transform to finally close in on the spectral density. Upon this we should have all requirements to start the investigation afterwards.

1.1 Unitary Matrices

Let's begin with a definition that will be relevant in later chapters. The index T marks the transpose of a matrix. As common in a lot of literature, I_n denotes the identity matrix of size n .

Definition 1 (Orthogonal matrix). Let A be a real, square matrix of size n . Then A is called *orthogonal* if $A^T \cdot A = I_n$.

For the entirety of this thesis, let A always be a complex, square matrix of size n unless stated otherwise. Note that A^* is *conjugate transpose* of the matrix A with all of its entries complex conjugated and transposed.

Definition 2 (Unitary matrix). A matrix A is called *unitary* if $A^* \cdot A = I_n$.

We will oftentimes denote unitary matrices by using U as a reference. It is easy to see that orthogonal matrices are a special case of unitary matrices, since $A^T = A^*$ for all real matrices.

Now, let's assume we have a unitary matrix U and are trying to find its eigenvalues. That means we have to solve the equation

$$U \cdot v = \lambda \cdot v \tag{1.1}$$

for a complex vector $v \neq \mathbf{0}$ of size n and a scalar $\lambda \in \mathbb{C}$. The complex conjugate of this equation is

$$v^* \cdot U^* = v^* \cdot \lambda^* = \lambda^* \cdot v^* \tag{1.2}$$

Put together, we calculate

$$\begin{aligned}
v^* \cdot v &= v^* \cdot U^* \cdot U \cdot v \\
&= v^* \cdot \lambda^* \cdot \lambda \cdot v \\
&= \lambda^* \cdot \lambda \cdot v^* \cdot v \\
&= |\lambda|^2 \cdot v^* \cdot v
\end{aligned}$$

Since we have that $v \neq \mathbf{0}$ it follows that $v^* \cdot v \neq 0$. Therefore, we can divide by $v^* \cdot v$ to obtain

$$1 = |\lambda|^2 = |\lambda| \quad (1.3)$$

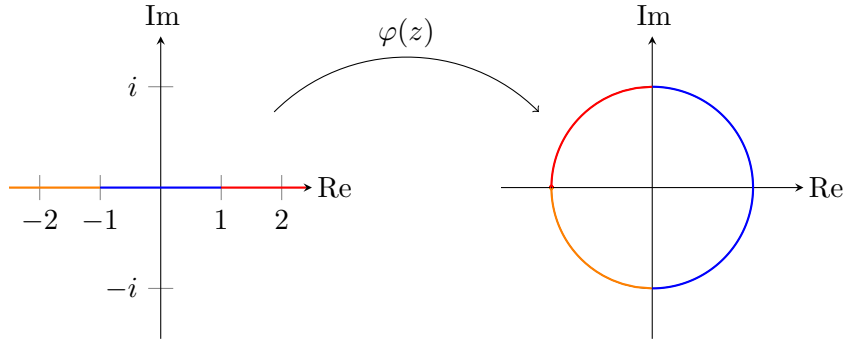
meaning that all eigenvalues of unitary matrices have a length of 1 and are situated on the unit circle. For orthogonal matrices, this means their eigenvalues are either 1 or -1 . This is an important property, as it justifies that we can make use of the Cayley transform introduced in the following section.

1.2 Cayley Transform

The Cayley transform or Cayley transformation is given by the simple function

$$\varphi(z) = (i - z)(i + z)^{-1}$$

This function maps the real line to the unit circle, and more specifically, the interval $[-1, 1]$ to the semi circle $\{z = e^{i\theta} : \theta \in [-\pi/2, \pi/2]\}$ as shown below



This will be relevant later, as we can then use φ to transform unitary matrices into symmetric ones and vice versa. Now, let's look how the spectral density is defined in the next section.

1.3 Spectral Density

Bibliography

- [1] CHRISTIAN BÄR, *Lineare Algebra und analytische Geometrie*, Springer Spektrum 2018
- [2] LIN LIN, YOUSSEF SAAD AND CHAO YANG, *Approximating Spectral Densities of Large Matrices*, <https://arxiv.org/pdf/1308.5467v2>
5. Oktober 2014
- [3] G. H. GOLUB UND C. F. VAN LOAN, *Matrix Computations, 4th Edition*, Johns Hopkins University Press, Baltimore, MD, 3rd ed., 2013
- [4] R. D. RICHTMYER, *Principles of advanced mathematical physics*, vol 1, Springer Verlag, New York, 1981