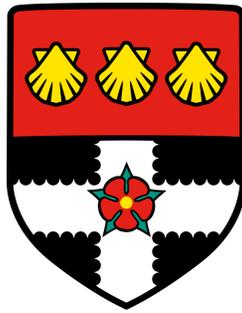


Spectra of Indefinite Linear Operator Pencils



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Abstract

In recent years, there has been a rapid growth of interest in spectral properties of non-self-adjoint operators and operator pencils. This thesis is concerned with indefinite self-adjoint linear pencils which lead to a special class of non-self-adjoint spectral problems. These problems are not well understood, and, in general, many sign-indefinite problems which are trivial to state require some highly non-trivial analysis.

We look at indefinite linear pencil problems from the perspective of a two parameter eigenvalue problem. We derive localisation results for real eigenvalues and present several examples. We also use different approaches to obtain estimates of non-real eigenvalues, supported by a large number of numerical experiments. Additionally, these experiments lead to various open questions and conjectures.

Declaration

I confirm that this is my own work and that the use of all material from other sources has been properly and fully acknowledged.

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Chapter 1

Introduction

Spectral theory is one of the richest fields in mathematics and one can find its various applications in classical as well as quantum physics, such as in the study of control theory [35], the physics of musical instruments [24, 33], quantum mechanics [39] and signal processing [57], see [74] for more details.

The spectral theory of linear self-adjoint operators was first presented by D. Hilbert in his famous papers (1904-1910). Following this, the abstract concepts of Hilbert spaces and linear operators were developed by von Neumann whose work was used to build quantum mechanics, which was created by Jordan, Schrödinger, Dirac, and others. Since then, self-adjoint operators have been extensively studied in the literature (see [69, 75] for a detailed survey). This was in part due to the needs of quantum mechanics, where fundamental properties such as momentum, position, and the Hamiltonian are expressed in this form. Today, many books can be found in this field (e.g. [13, 21]).

On the other hand, G. D. Birkhoff initiated the basics on eigenfunction expansions for non-self-adjoint operators between 1908 and 1913. Although his works were written during the same period as Hilbert's papers, the first abstract results in this field appeared in the literature in 1951, written by M. V. Keldys. There are many authors who made important contributions to the field, including Kato, Wolf, Gohberg, Krein and Langer. For more detailed historical information, see [16, 20, 75] and references therein. Non-self-adjoint operators have a wide range of physical applications, they arise, for instance, in the study of biological systems [59], in the exploration of resonance phenomena [56], describing the motion and oscillation of viscous fluids [36], the optical singularities of crystals [9], the optical model of nuclear scattering [8], and others.

Hermitian systems describe time-dependent systems which conserve the energy, while non-Hermitian systems do not. Examples of such non-Hermitian systems appear, for example, in friction problems and inelastic scattering problems. For recent advances and open problems in quantum physics related to non-self-adjoint operators, see [6, 7, 30].

Although the theory of non-self-adjoint operators is still under development, it already has a variety of applications in different fields, and the theory is far from complete.

This thesis will focus on self-adjoint linear operator pencils which lead to a class of non-self-adjoint operators. Before going into the details of this relation, the general theory of operator pencils will be discussed in the next section. Throughout the thesis, \mathcal{H} denotes a finite-dimensional, complex Hilbert space, equipped with inner product $\langle \cdot, \cdot \rangle$ such that $\langle a\mathbf{u}, b\mathbf{v} \rangle = a\bar{b}\langle \mathbf{u}, \mathbf{v} \rangle$, $\mathbf{u}, \mathbf{v} \in \mathcal{H}$, $a, b \in \mathbb{C}$. We will be working with operators acting on \mathcal{H} , and therefore they are bounded. The identity operator on \mathcal{H} will be denoted by I . We denote by $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ the space of all bounded operators from \mathcal{H}_1 to \mathcal{H}_2 . If $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$, then we use the short form $\mathcal{B}(\mathcal{H}) = \mathcal{B}(\mathcal{H}, \mathcal{H})$. Capital bold letters (e.g. \mathbf{X}) represent block matrices, small bold letters (e.g. \mathbf{u}) represent vectors. A^T and A^* represent the transpose and the adjoint of A , respectively. We denote by $\text{diag}(\lambda_1, \dots, \lambda_m)$ a diagonal matrix with entries $\lambda_1, \dots, \lambda_m$.

1.1 Operator pencils

Operator pencils (or *polynomial operator pencils*) are a family of operators depending on a parameter, that is, operator polynomials of the form

$$\mathcal{P} = \mathcal{P}(\lambda) = A_0 + \lambda A_1 + \lambda^2 A_2 + \dots + \lambda^k A_k,$$

where λ is a spectral parameter and A_0, \dots, A_k are linear operators acting on a finite-dimensional Hilbert space \mathcal{H} . If the operator coefficients are self-adjoint; i.e.

$$A_j = (A_j)^*, \quad j = 0, 1, \dots, k,$$

then such a family is called a self-adjoint operator pencil.

A complex number λ_0 is said to be an eigenvalue of the pencil \mathcal{P} if $\mathcal{P}(\lambda_0)$ is not invertible, or equivalently if

$$\mathcal{P}(\lambda_0)\mathbf{u} = 0$$

has a non-zero solution $\mathbf{u} \in \mathcal{H} \setminus \{\mathbf{0}\}$. The set of all eigenvalues of the pencil \mathcal{P} is called the spectrum of \mathcal{P} , which will be denoted by $\text{Spec}(\mathcal{P})$. Moreover, $\text{Spec}(\mathcal{P})$ coincides with the set

$$\text{Spec}(\mathcal{P}) = \{\lambda \in \mathbb{C} : \det(\mathcal{P}) = 0\}.$$

If one considers the simplest case $\mathcal{P}(\lambda) = A - \lambda I$ where A is a single operator and I is the identity operator, then the pencil problem is equivalent to the spectral problem of a single

operator A . The spectrum $\text{Spec}(A)$ of a linear operator A is the set of $\lambda \in \mathbb{C}$ such that the operator $A - \lambda I$ is not invertible, which is the same as that of the pencil $\mathcal{P}(\lambda) = A - \lambda I$.

For a bounded linear operator T on a Hilbert space \mathcal{H} , we define the operator norm of T as

$$\|T\| = \sup\{|\langle T\mathbf{x}, \mathbf{y} \rangle| : \mathbf{x}, \mathbf{y} \in \mathcal{H}, \|\mathbf{x}\| = \|\mathbf{y}\| = 1\}.$$

The spectral theory of operator pencils has a rich and long history. Pioneering works were undertaken by Tamarkin, Keldysh, Krein, Langer, Shkalikov and others (see [45] for a historical survey). In recent years, it has been a very active research area from both a theoretical and a numerical point view. It has many applications, for instance to control theory [15], vibrating structures [60, 73], mathematical physics and quantum mechanics [6, 62] and more recently electron waveguide in graphene [22, 28, 42]. Several other applications of operator pencils can also be found in [45].

1.2 Indefinite linear pencils

This thesis is devoted to the theory of indefinite linear pencils. We begin by comparing the systems which have a definite or indefinite operator A . A self-adjoint operator $A : \mathcal{H} \rightarrow \mathcal{H}$ is said to be *positive definite* if and only if all its eigenvalues are positive, or equivalently

$$\langle A\mathbf{x}, \mathbf{x} \rangle > 0$$

for every non-zero vector $\mathbf{x} \in \mathcal{H}$. The *negative definite* operators are defined analogously. A linear operator A is called *indefinite* if there exist $\mathbf{x}, \mathbf{y} \in \mathcal{H}$ for which

$$\langle A\mathbf{x}, \mathbf{x} \rangle > 0, \quad \langle A\mathbf{y}, \mathbf{y} \rangle < 0.$$

One often finds a generalised spectral problem for a pair of self-adjoint operators A, B acting in a Hilbert space \mathcal{H} as: find $\lambda \in \mathbb{C}$ such that

$$A\mathbf{u} = \lambda B\mathbf{u}. \tag{1.1}$$

Suppose that $B > 0$ (i.e. B is positive definite), then there exists $\sqrt{B} > 0$ and, by a change of variables,

$$\mathbf{v} = B^{1/2}\mathbf{u} \quad \Leftrightarrow \quad B^{-1/2}\mathbf{v} = \mathbf{u},$$

so that the problem (1.1) becomes

$$A\mathbf{u} = \lambda B\mathbf{u} \quad \Leftrightarrow \quad AB^{-1/2}\mathbf{v} = \lambda B^{1/2}\mathbf{v} \quad \Leftrightarrow \quad B^{-1/2}AB^{-1/2}\mathbf{v} = \lambda\mathbf{v}.$$

Now, $B^{-1/2}AB^{-1/2}$ is a product of three self-adjoint operators and it is self-adjoint since $(CDE)^* = E^*D^*C^*$, therefore all its eigenvalues are real.

If $A > 0$, then by setting $\mu = 1/\lambda$ in (1.1) yields

$$B\mathbf{u} = \mu A\mathbf{u},$$

and then, applying to the same reasoning for $\sqrt{A} > 0$, the spectral problem can be reduced to one for a self-adjoint operator $A^{-1/2}BA^{-1/2}$.

If $B < 0$ (similarly $A < 0$), switching the problem to

$$(-A)\mathbf{u} = \lambda(-B\mathbf{u}),$$

and since $-B > 0$ (or $-A > 0$), the problem can be modified in the same way and it follows that the spectrum is real.

If both A, B are sign-definite, then the problem (1.1) is called sign-definite as well. If only one of A, B is sign-definite, then (1.1) is called semi-definite (but still reduces to a self-adjoint spectral problem). In the general case when A and B are *sign-indefinite* (or *indefinite*), the same tricks cannot be applied, and in this case (1.1) is called indefinite.

If B is invertible, then the problem (1.1) can be reduced to

$$B^{-1}A\mathbf{u} = \lambda\mathbf{u}.$$

However, in general, B^{-1} and A do not necessarily commute, that is,

$$(B^{-1}A)^* = AB^{-1} \neq B^{-1}A,$$

thus the operator $B^{-1}A$ may not be self-adjoint. Therefore there may be some complex eigenvalues in the spectrum.

The problem (1.1) is the spectral problem for the linear pencil

$$\mathcal{P}(\lambda) = A - \lambda B, \tag{1.2}$$

where A, B is a pair of self-adjoint operators acting in a Hilbert space \mathcal{H} and $\lambda \in \mathbb{C}$. A pencil of the form (1.2) with both A and B self-adjoint is called a self-adjoint pencil. We are interested in the case when both A and B are sign-indefinite. We always assume that B is invertible so that the spectrum of the pencil $\mathcal{P}(\lambda)$ coincides with that of the operator $B^{-1}A$.

The difficulty is that standard operator theoretical methods available for the self-adjoint case, for instance the classical variational principles and the spectral theorem, do not readily apply and very little information can be deduced about non-real eigenvalues from the general theory, see, for instance, the next result.

Lemma 1.2.1. *Suppose that \mathbf{u} is an eigenvector corresponding to the eigenvalue λ of a self-adjoint pencil $A - \lambda B$. If $\lambda \in \mathbb{C} \setminus \mathbb{R}$, then $\langle B\mathbf{u}, \mathbf{u} \rangle = 0$ and thus $\langle A\mathbf{u}, \mathbf{u} \rangle = 0$.*

Proof. Multiplying (1.1) with \mathbf{u} from both sides, we get

$$\langle A\mathbf{u}, \mathbf{u} \rangle = \lambda \langle B\mathbf{u}, \mathbf{u} \rangle.$$

We know that $\langle A\mathbf{u}, \mathbf{u} \rangle$ and $\langle B\mathbf{u}, \mathbf{u} \rangle$ are real and therefore taking the imaginary part of both sides we obtain

$$0 = \langle B\mathbf{u}, \mathbf{u} \rangle \text{Im}(\lambda),$$

which implies that $\lambda \in \mathbb{R}$ or $\langle B\mathbf{u}, \mathbf{u} \rangle = 0$. The result follows since we consider $\lambda \in \mathbb{C} \setminus \mathbb{R}$. \square

The main objective of this thesis is to study the spectral properties of some sign-indefinite self-adjoint linear operator pencils. There are not many examples of such pencils in the literature. Similar problems appeared in [19, 22, 42, 46] where it was shown that many sign-indefinite problems which are trivial to state, require highly non-trivial analysis. One cannot obtain good bounds and estimates on eigenvalues by purely functional analytic methods.

1.3 Key results and outline of the thesis

Chapter 2 will provide the necessary background from functional analysis. We begin this chapter with a brief overview of block matrices. The statements given in Section 2.1 are already known, however we will use them in Chapter 4 to obtain information about the eigenvalues of a pencil problem.

In Section 2.2 we present a review of the known Gershgorin-type results. Gershgorin's method [25] is a well-known method for the localisation of the eigenvalues of a complex square matrix. His result is usually referred to as the Gershgorin (circle) Theorem, and states that all the eigenvalues of a matrix with complex entries are contained in a union of disks. The centre of the disks are the diagonal entries of the matrix, and the radii are given by the row sum of the absolute values of the non-diagonal entries. Namely, the result is given as follows.

Theorem 1.3.1 (Gershgorin (circle) Theorem, [25, 79]). *Let $a_{i,j}$ denote the (i, j) -th element of the matrix A , that is, $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$, $n \geq 2$. Then*

$$\text{Spec}(A) \subseteq \mathcal{G}(A) := \bigcup_{i=1}^n \mathcal{G}_i(A),$$

where

$$\mathcal{G}_i(A) := \{\lambda \in \mathbb{C} : |\lambda - a_{i,i}| \leq r_i(A)\}, \quad (1.3)$$

and $r_i(A)$ denotes the i -th deleted absolute row sum of A , i.e.

$$r_i(A) = \sum_{j \in J_i} |a_{i,j}|, \quad J_i = \{1, 2, \dots, n\} \setminus \{i\}. \quad (1.4)$$

Section 2.2 contains a collection of theorems related to Gershgorin-type results on the localisation of eigenvalues. We shall apply these results to a particular problem and illustrate some of them in Section 4.5.3. We will finish this subsection by giving a new result; a Gershgorin-type localisation for a two-parameter eigenvalue problem (see Corollary 2.2.16).

In Section 2.3, we will briefly present the general theory of orthogonal polynomials. We will then discuss some properties of Chebyshev polynomials of the second kind, which are our main interest in this section. We will study the spectral properties of the matrix whose determinant leads to Chebyshev polynomials of the second kind. Our main focus in the last part of this section will be on ratio asymptotic results given by Simon [66]. We will recall some of his results and apply them to a particular problem in Section 4.5.2.

There are also other approaches to sign-indefinite pencils, for instance, Krein spaces, numerical range (NR) and block numerical range (BNR). We conducted some numerical investigations on a linear pencil problem. However, they did not produce much information, therefore we do not pursue them in this thesis and we omitted the plots and the investigations we carried out. A comprehensive introduction to Krein spaces is provided in [5, 14, 27, 34, 40] and to NR and BNR in [43, 47, 61, 63, 75, 76].

In **Chapter 3**, we focus on a two-parameter eigenvalue problem, and most results of this chapter have been published in [41]. The main motivation of this chapter comes from a particular example of a finite-dimensional, sign-indefinite, self-adjoint linear pencil, studied by Davies and Levitin [19]. We consider the linear pencil problem in a more general setting, and under reasonable restrictions, we state localisation theorems for the eigenvalues.

We start the chapter by surveying the work of Davies and Levitin [19], and then introduce and study a two-parameter eigenvalue problem. Namely, let $m, n \in \mathbb{N}$ and $N = m+n$, then Davies and Levitin [19] consider the linear operator pencil

$$\mathcal{A}_c = \mathcal{A}_c(\lambda) := H_c^{(N)} - \lambda S_{m,n}, \quad (1.5)$$

In here, A and D are self-adjoint operators in the Hilbert spaces \mathcal{H}_1 , \mathcal{H}_2 , respectively, and C is a linear operator from \mathcal{H}_2 to \mathcal{H}_1 , then one can re-write the two-parameter eigenvalue problem (1.7) as

$$\mathbf{M}(\alpha, \beta) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} A - \alpha & C \\ C^* & D - \beta \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}, \quad (1.9)$$

where $A - \alpha$ and $D - \beta$ are shorthand for $A - \alpha I$ and $D - \beta I$, respectively.

Remark 1.3.2. There may be other points $(\alpha, \beta) \in \mathbb{C}^2$ where \mathbf{M} does not have a bounded inverse in general. However, we study the eigenvalues of \mathbf{M} and Spec_p stands for point spectrum.

Now, let us investigate the connection between a two-parameter eigenvalue problem (1.9) and a linear pencil problem (1.2). Consider the self-adjoint, linear matrix pencil

$$(\mathbf{L} + cI - \lambda \mathbf{S})\mathbf{x} = \mathbf{0}, \quad (1.10)$$

where \mathbf{L} is given by (1.8) and

$$\mathbf{S} = \begin{pmatrix} I & \\ & -I \end{pmatrix}.$$

Further λ is a spectral parameter and $c \in \mathbb{R}$ is fixed. Then (1.10) can be re-written as a generalised eigenvalue problem

$$\begin{pmatrix} A + c & C \\ C^* & D + c \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} I & \\ & -I \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \quad (1.11)$$

which is equivalent to

$$\begin{pmatrix} A + c - \lambda & C \\ C^* & D + c + \lambda \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}. \quad (1.12)$$

In addition, the problem (1.11) is also equivalent to the non-self-adjoint problem

$$\begin{pmatrix} A + c & C \\ -C^* & -D - c \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}. \quad (1.13)$$

Then it can be seen from (1.12) that any linear pencil problem of the form (1.10) (or a non-self-adjoint problem of the form (1.13)) relates to the two-parameter eigenvalue of the form (1.9) by setting

$$\alpha = \lambda - c; \quad \beta = -\lambda - c. \quad (1.14)$$

Indeed, it can be said that Davies and Levitin [19] considered the two-parameter eigenvalue problem (1.9) in the case when $\mathbf{S} = S_{m,n}$, $A = H_0^{(n)}$, $D = H_0^{(m)}$, $(C)_{n,1} = 1$ and all

other entries of C are zeros. In Section 3.2, the problem (1.9) is attacked in a more general setting; we consider the case when A, D are self-adjoint operators and C is rank one, and we obtain localisation results on the real pair-eigenvalues of the two-parameter eigenvalue problem. The main results (Theorem 3.3.6 and its special case Theorem 3.3.4) will be given in Section 3.3. For simplicity, we omit the statement of our main results here and we give an illustrative example instead. For instance, let

$$A = D = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix},$$

then the pair-eigenvalues of M lie in a union of rectangular regions in the (α, β) -plane. In Figure 1.1, we illustrate the region (light-gray shaded area) which contains the real spectrum of M (blue lines). Boundaries of the region and some special cases will be explained later in this chapter.

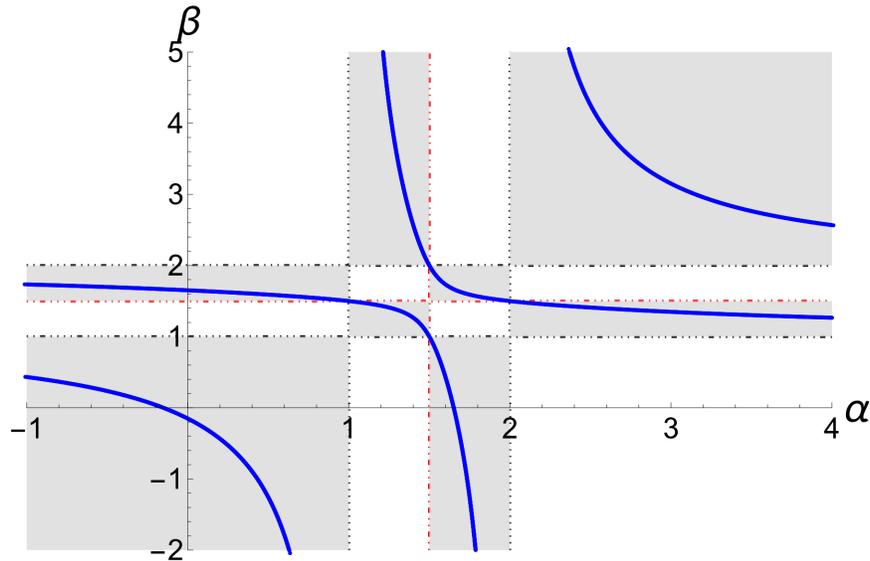


Figure 1.1: In the (α, β) -plane, blue lines are the real pair-eigenvalues of M .

The rest of this chapter is devoted to the study of a two-parameter eigenvalue problem. Throughout this chapter, we deal with mainly the real pair-eigenvalues of a two-parameter eigenvalue problem. We focus on the non-real pair-eigenvalues of the problem only in Section 3.7. First, we start Section 3.2 by describing the general concept of a two-parameter eigenvalue problem. Then in Section 3.3 after imposing some restrictions and notation, we state the main results of this chapter concerning the real pair-eigenvalues of M , namely Theorem 3.3.6 and its special case Theorem 3.3.4. In Section 3.4 we briefly discuss some auxiliary results for a special class of problems and subsequently we give

the proofs of the main results in Section 3.5. Afterwards, we give several examples to illustrate the special cases in Section 3.6.

We conclude the chapter with a discussion of the non-real pair-eigenvalues of a two-parameter eigenvalue problem. In general, there are infinitely many $\beta \in \mathbb{C}$ for every $\alpha \in \mathbb{C} \setminus \text{Spec}(A)$. Thus we shall limit our attention to those that satisfy

$$\text{Im}(\alpha + \beta) = 0.$$

Therefore, we set

$$\widetilde{\text{Spec}}(\mathbf{M}) := \text{Spec}_p(\mathbf{M}) \cap \{(\alpha, \beta) \in \mathbb{C}^2 : \text{Im}\alpha + \text{Im}\beta = 0\}.$$

First, we locate the collision points of the real eigenvalues (or double eigenvalues) in terms of the first derivative of $\beta(\alpha)$ with respect to α and we state the result in Lemma 3.7.3. Another major result of our investigation concerning the non-real pair-eigenvalues of \mathbf{M} is given in Theorem 3.7.4. Using asymptotic analysis, we prove that as $\|C\|$ diverges to infinity there exists a family of non-real pair eigenvalues which approximately lies on a circle in the complex plane. The centre and the radius of this circle will be explained in Section 3.7.1, including illustrative examples.

We estimate the real eigenvalues of the pencil \mathcal{A}_c by looking at a corresponding two-parameter eigenvalue problem. We also obtain partial information about the non-real pair-eigenvalues of the problem which we will study in detail in Section 3.7. In addition, we obtain some minimal information about the collisions of the real eigenvalues (i.e. double eigenvalues). Therefore, we need to look at the concrete example again so as to gain more insight about the open problems from [19].

We note that in our publication [41] we focus on the two-parameter eigenvalue problem (1.9) in the case when $\dim \mathcal{H}_1 = \dim \mathcal{H}_2$, whereas in this chapter, we extend our results to a more general setting. In addition, Lemma 3.5.5, Lemma 3.7.1 and Theorem 3.7.4 are new, and do not appear in the paper [41].

In **Chapter 4** we turn our attention to the linear pencil problem (1.5). We shall only consider the case when $m = n$ in this chapter. By rephrasing the work of Davies and Levitin [19], we are able to gain a new perspective. First, we look at the characteristic equation of the pencil \mathcal{A}_c in Section 4.1 which can be written in several ways, one of which is using iterative functions that turn out to be related to ratios of Chebyshev polynomials of the second kind U_n . In Section 4.1.1, we shall deduce the characteristic equation of the pencil \mathcal{A}_c explicitly and give explicit expressions for the eigenfunctions of the pencil \mathcal{A}_c in terms of the Chebyshev polynomials of the second kind, see Lemma 4.1.3.

We will frequently use the following substitution

$$\lambda - c := z + \frac{1}{z}, \quad \lambda + c := w + \frac{1}{w}, \quad (1.15)$$

where λ is an eigenvalue of the pencil \mathcal{A}_c and $z, w \in \mathbb{C}$. Then each λ corresponds to two values of z and two values of w , which are the solutions of the quadratic equations

$$\begin{aligned} z^2 - (\lambda - c)z + 1 &= 0, \\ w^2 - (\lambda + c)w + 1 &= 0, \end{aligned}$$

respectively. Using (1.15), Davies and Levitin [19] gave another form of the characteristic equation, and we quote some of their results in Section 4.1.2. In Section 4.1.3, the pencil problem will be re-written in the basis of the eigenfunctions $\{\psi_j\}$ of $H_0^{(n)}$.

Numerical experiments suggest that the eigenvalues of a sign-indefinite self-adjoint pencil often lie on or under a set of curves. Davies and Levitin [19] proved that this is true in some cases, and determined the curve asymptotically which bounds the spectrum of \mathcal{A}_c when $c \neq 0$. Nevertheless, the crucial step in the proof was the following conjecture.

Conjecture 1.3.3 ([19, Conjecture 5.3]). *Let $c > 0$ and $m = n$. If λ is a non-real eigenvalue of \mathcal{A}_c , then*

$$|\lambda \pm c| < 2, \quad (1.16)$$

and therefore

$$|\operatorname{Re}(\lambda)| < 2 - c. \quad (1.17)$$

Conjecture 1.3.3 is still open. We have verified this conjecture numerically for a wide range of n and c , and we will give numerical experiments to support this conjecture throughout this thesis. One of these experiments is illustrated in Figure 1.2, showing the complicated interplay between $\max_{\lambda \in \operatorname{Spec}(\mathcal{A}_c) \setminus \mathbb{R}} \{|\lambda + c|, |\lambda - c|\}$ and c . We see in the figure that the maximum value of $|\lambda \pm c|$ never exceeds two.

We will look at the pencil problem from different angles and we will see that there are several ways to reformulate Conjecture 1.3.3. To make these reformulations more accessible as a whole, we summarize them as follows.

Theorem 1.3.4. *Conjecture 1.3.3 is satisfied if and only if any of the following statements hold:*

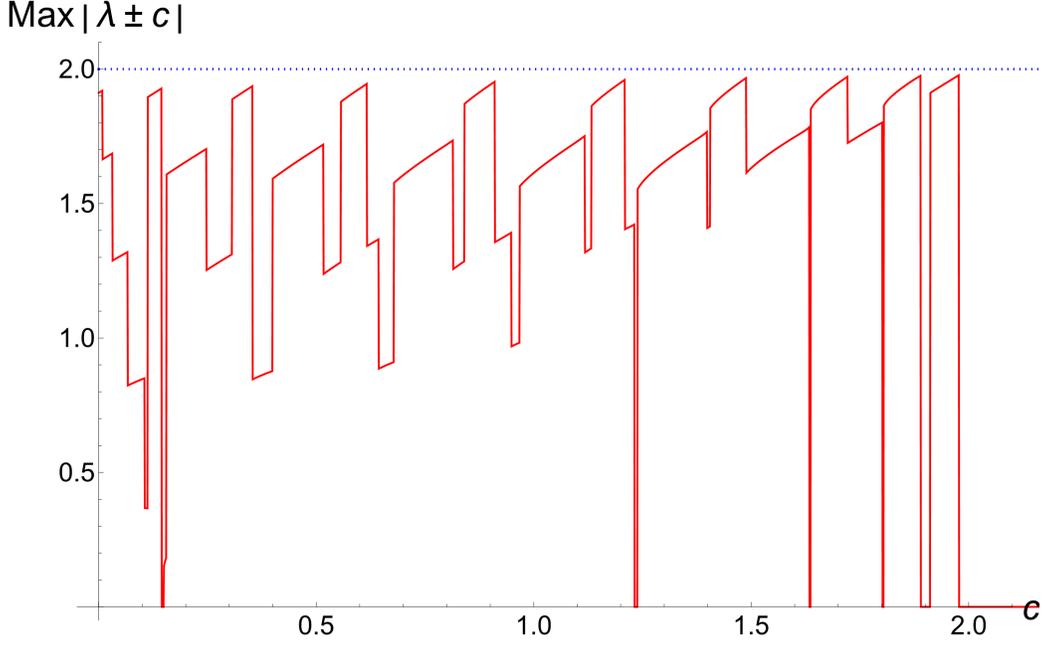


Figure 1.2: For $n = 10$, $\max\{|\lambda + c|, |\lambda - c|\}$ (red lines) among all non-real eigenvalues of \mathcal{A}_c is drawn as c ranges from 0 to 2 with the step-size 0.001 and the constant line at 2 (blue dotted lines).

(i) Consider a two-parameter eigenvalue problem $\mathbf{M}(\alpha, \beta)$ defined by (1.9) with $A = D = H_0^{(n)}$ and $C = C^*$ with $(C)_{nn} = 1$ and all other entries of C are zeros. Then

$$\widetilde{\text{Spec}}(\mathbf{M}) \setminus \mathbb{R}^2 \subset \{(\alpha, \beta) : |\alpha|, |\beta| < 2\}.$$

(ii) Let $\sigma, \tau \in \mathbb{C}$, $\text{Im}(\sigma) = \text{Im}(\tau) > 0$. If, for some $n \in \mathbb{N}$,

$$U_n(\sigma)U_n(\tau) + U_{n-1}(\sigma)U_{n-1}(\tau) = 0, \quad (1.18)$$

then $|\sigma| < 1$ and $|\tau| < 1$.

(iii) Let $\tilde{F}_n : \mathbb{C} \rightarrow \mathbb{C}$, $n \geq 1$ denote the sequence of iteratively defined rational functions

$$\tilde{F}_{n+1}(\zeta) = \zeta - \frac{1}{\tilde{F}_n(\zeta)}, \quad \tilde{F}_1(\zeta) = \zeta, \quad \zeta \in \mathbb{C}.$$

Then any solution $(\sigma, \tau) \in \mathbb{C}^2$ of

$$\tilde{F}_n(\sigma)\tilde{F}_n(\tau) = -1, \quad \text{Im}(\sigma) = \text{Im}(\tau) > 0,$$

has both $|\sigma| < 2$ and $|\tau| < 2$.

(iv) Let $G_n : \mathbb{C} \rightarrow \mathbb{C}$, $n \geq 1$ denote the family of meromorphic functions

$$G_n(\xi) := \frac{\xi^{n+1} - \xi^{-n-1}}{\xi^n - \xi^{-n}}.$$

Let $z, w \in \mathbb{C} \setminus \mathbb{R}$ such that $|z|, |w| > 1$. Then any solutions z, w of

$$G_n(z)G_n(w) = -1,$$

satisfy

$$z, w \in \mathcal{Z}_1 \cup \mathcal{Z}_2 \tag{1.19}$$

where

$$\mathcal{Z}_1 := \left\{ \zeta \in \mathbb{C} : |\zeta| > 1 \text{ and } |\zeta - i| < \sqrt{2} \right\}, \quad \mathcal{Z}_2 := \left\{ \zeta \in \mathbb{C} : |\zeta| > 1 \text{ and } |\zeta + i| < \sqrt{2} \right\}.$$

(v) Let $\mathbf{A}_c = S_{n,n}^{-1} H_c^{(N)}$. Then

$$\text{Spec}(\mathbf{A}_c) \setminus \mathbb{R} \subset \left(\bigcup_{i=1}^n \mathcal{G}_i(\mathbf{A}_c) \right) \cap \left(\bigcup_{j=n+1}^{2n} \mathcal{G}_j(\mathbf{A}_c) \right).$$

We prove most of these reformulations in Section 4.2. Only two of these equivalences were deduced by Davies Levitin [19], namely Theorem 1.3.4(ii) and (iii). We prove these reformulations in Section 4.2.1. The rest of the reformulations are new. We give a proof of Theorem 1.3.4(i) in Section 3.7. We will derive Theorem 1.3.4(iv) in Section 4.2.2 and verify Theorem 1.3.4(v) in Section 4.2.3.

In Section 4.3 we give a proof of Conjecture 1.3.3 in the case $n = 2$ and $n = 3$. Although we can prove the conjecture explicitly, the proof involves very long computations for even small matrices. In Section 4.4, we describe the asymptotic behaviour of the non-real eigenvalues of the pencil \mathcal{A}_c as the parameter c tends to zero.

Our purpose in Section 4.5 is to apply useful methods mentioned in Chapter 2 to our problem. We begin this section with a brief discussion of the pencil problem in a block operator setting. The main objective is to show the difficulty of the problem.

As mentioned in Theorem 1.3.4(ii), Conjecture 1.3.3 can be reformulated as a result involving Chebyshev polynomials of the second kind U_n . This statement is apparently a new statement for Chebyshev polynomials. One approach is to treat the system as the ratios of Chebyshev polynomials of the second kind. It is still an open question to estimate the ratio for orthogonal polynomials of finite index. In Section 4.5.2, first we apply the ratio asymptotic results given in Section 2.3.4 to the ratio $U_n(\zeta)/U_{n-1}(\zeta)$. Afterwards, we investigate various properties of this finite ratio and deduce some bounds on this ratio. Although these bounds are not sufficient to prove the conjecture, we believe that they are still useful. Most of these results in this subsection are joint with Sabine Bögli

(unpublished). Although the reformulations given in Theorem 1.3.4(ii) and (iii) were already deduced by Davies and Levitin [19], they haven't studied the ratio of orthogonal polynomials, and we remark that our investigation is a new approach.

Another form of Conjecture 1.3.3 is given in terms of Gershgorin circles as in Theorem 1.3.4(v). When we apply Gershgorin's Theorem to our problem, we will see in Section 4.2.3 that all the eigenvalues of \mathcal{A}_c lie in the union of all disks, whereas we claim that the non-real eigenvalues of \mathcal{A}_c lie in the intersection of two regions. In Section 4.5.3, we will apply various Gershgorin-type results mentioned in Section 2.2 to our pencil problem. We will see that there is no such Gershgorin-type region which contains only the non-real eigenvalues of a matrix. We tried but failed to obtain such bounds, and therefore we omitted our calculations. Instead, we will investigate and illustrate some of the known results, and we will see that a very few of them give a better bound than Gershgorin Theorem when applied to our problem. We end this chapter by applying the Gershgorin-type localisation for a two-parameter eigenvalue problem to our problem, and we look at the Gershgorin's result under the change of variables (1.15).

Chapter 5 focuses on localisation of the non-real eigenvalues from different perspectives. We mention some heuristics based on numerical experiments. In Section 5.1, we explain the dynamics of the eigenvalues of the pencil \mathcal{A}_c as the parameter c changes. There is a fascinating dynamics of real eigenvalues colliding to form a pair of complex-conjugate eigenvalues emerging into the complex plane, and the reverse collisions of complex eigenvalues. We illustrate these collisions (or jumps) which occur in the first quadrant of the complex plane in Table 5.1. In Section 5.2, we illustrate some interesting phenomena for the non-real pair-eigenvalues of a two parametric eigenvalue problem. In Section 5.3, we investigate double eigenvalues of the pencil \mathcal{A}_c . One would see an interesting behaviour if one superimposes the double eigenvalues of \mathcal{A}_c for the values of n , see Figure 5.6. In addition, we count the number of double eigenvalues which lie in a certain location. Numerical evidence suggests that for c between 0 and 2, there are altogether $2n^2$ double λ -roots (conjectured), of which $2n$ are at the origin and the rest are non-zero.

Chapter 2

Background

In this chapter, we discuss some necessary background material from functional analysis. In Section 2.1, we review some properties of block matrices. Most of the results contained in this section are probably well-known, however these ideas will be used in Chapter 4. Section 2.2 contains a review of the well-known Gershgorin-type results, which we will apply in Section 4.5.3 to our problem and give a detailed discussion of their applications. In Section 2.3, we provide a brief overview of orthogonal polynomials before turning to a discussion of Chebyshev polynomials of the second kind. We will introduce some notation and basic terminology, and discuss some of the spectral properties of a matrix. We conclude this section with a brief survey of ratio asymptotics of orthogonal polynomials.

2.1 Block matrices

In this section, we shall discuss some properties of block (operator) matrices. Let

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \tag{2.1}$$

be a direct sum of complex Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$. A linear operator $\mathbf{X} \in B(\mathcal{H})$ always admits a block (operator) matrix representation

$$\mathbf{X} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \tag{2.2}$$

with linear operators $A_{ij} \in \mathcal{B}(\mathcal{H}_j, \mathcal{H}_i)$, $i, j = 1, 2$. Most of the time, we will be interested in the special case when $\dim \mathcal{H}_1 = \dim \mathcal{H}_2$, $A_{jj} = A_{jj}^*$, $j = 1, 2$, and either $A_{21} = -A_{12}$ or $A_{21} = -A_{12}^*$. In the rest of this section, we set \mathbf{X} as a 2×2 block matrix with respect to the decomposition (2.1) and review some of its spectral properties.

We start by considering a 2×2 matrix, and we will then generalise the result for a 2×2 block matrix. The following lemma establishes certain bounds on the eigenvalues of 2×2 matrices.

Lemma 2.1.1. Let $Y = \begin{pmatrix} a & b \\ -\bar{b} & d \end{pmatrix}$, where $a, d \in \mathbb{R}$, and $b \in \mathbb{C}$. If $\lambda \in \mathbb{C} \setminus \mathbb{R}$ is an eigenvalue of Y , then

$$\begin{aligned} |a - d| &< 2|b|, \\ |\operatorname{Re}(\lambda) - a| &\leq |b|, \\ |\operatorname{Re}(\lambda) - d| &\leq |b|, \\ |\operatorname{Im}(\lambda)| &\leq |b|. \end{aligned}$$

Proof. Set $\beta = a + d$ and $\gamma = ad + |b|^2$, then the elementary formula $\lambda^2 - \beta\lambda + \gamma = 0$ gives

$$\begin{aligned} \lambda &= \frac{a + d}{2} \pm \sqrt{\frac{(a + d)^2}{4} - ad - |b|^2} \\ &= \frac{a + d}{2} \pm \sqrt{\frac{(a - d)^2}{4} - |b|^2}. \end{aligned}$$

The assumption $\lambda \notin \mathbb{R}$ implies that $(a - d)^2/4 - |b|^2 < 0$ and hence $|a - d|/2 < |b|$. It also implies that $\operatorname{Re}(\lambda) = (a + d)/2$. Therefore

$$|\operatorname{Re}(\lambda) - a| = \left| \frac{a + d}{2} - a \right| = \frac{|a - d|}{2} < |b|,$$

and similarly

$$\begin{aligned} |\operatorname{Re}(\lambda) - d| &= \frac{|a - d|}{2} < |b|, \\ |\operatorname{Im}(\lambda)| &= \sqrt{|b|^2 - \frac{(a - d)^2}{4}} \Rightarrow |\operatorname{Im}(\lambda)| \leq |b|. \end{aligned}$$

□

Remark 2.1.2. Lemma 2.1.1 is analogous to Lemma 1.2.7 from [75].

The next result gives some information for the eigenvectors of a certain type of a block matrix.

Lemma 2.1.3. Let $\gamma \in \mathbb{R}$. If $\lambda \in \mathbb{C} \setminus \mathbb{R}$ is an eigenvalue of

$$\mathbf{X}_\gamma = \begin{pmatrix} A_{11} - \gamma & A_{12} \\ -A_{12}^* & A_{22} + \gamma \end{pmatrix},$$

where $A_{jj} = A_{jj}^*$, $j = 1, 2$, then the corresponding eigenvectors $(\mathbf{u}, \mathbf{v})^T$ satisfy $\|\mathbf{u}\| = \|\mathbf{v}\|$. In addition,

$$|\operatorname{Im}(\lambda)| \leq \|A_{12}\|.$$

Proof. Consider the spectral problem

$$\begin{pmatrix} A_{11} - \gamma & A_{12} \\ -A_{12}^* & A_{22} + \gamma \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}.$$

Let $\lambda = x + iy$ where $x \in \mathbb{R}$ and $y \in \mathbb{R} \setminus \{0\}$. Then re-writing the problem as

$$\begin{cases} (A_{11} - \gamma)\mathbf{u} + A_{12}\mathbf{v} &= (x + iy)\mathbf{u}, \\ -A_{12}^*\mathbf{u} + (A_{22} + \gamma)\mathbf{v} &= (x + iy)\mathbf{v}, \end{cases}$$

and multiplying the first equation by \mathbf{u} and the second by \mathbf{v} gives

$$\begin{cases} \langle A_{11}\mathbf{u}, \mathbf{u} \rangle - \gamma\|\mathbf{u}\|^2 + \langle A_{12}\mathbf{v}, \mathbf{u} \rangle &= (x + iy)\|\mathbf{u}\|^2, \\ -\langle A_{12}^*\mathbf{u}, \mathbf{v} \rangle + \langle A_{22}\mathbf{v}, \mathbf{v} \rangle + \gamma\|\mathbf{v}\|^2 &= (x + iy)\|\mathbf{v}\|^2. \end{cases} \quad (2.3)$$

Considering the imaginary parts of (2.3), we get

$$\begin{cases} -y\|\mathbf{u}\|^2 + \operatorname{Im}\langle A_{12}\mathbf{v}, \mathbf{u} \rangle &= 0 \\ \operatorname{Im}\langle A_{12}^*\mathbf{u}, \mathbf{v} \rangle + y\|\mathbf{v}\|^2 &= 0, \end{cases} \quad (2.4)$$

and since $\langle A_{12}\mathbf{v}, \mathbf{u} \rangle = \overline{\langle A_{12}^*\mathbf{u}, \mathbf{v} \rangle}$, summing the two equations in (2.4) gives the first result.

In addition, we have from (2.4) that

$$|y| = \frac{|\operatorname{Im}\langle A_{12}\mathbf{v}, \mathbf{u} \rangle|}{\|\mathbf{u}\|^2} \leq \frac{\|A_{12}\mathbf{v}\|\|\mathbf{u}\|}{\|\mathbf{u}\|^2}, \quad (2.5)$$

and since $\|\mathbf{u}\| = \|\mathbf{v}\|$, we obtain $|y| \leq \|A_{12}\|$. \square

Remark 2.1.4. Note that we have the relation

$$\lambda \in \operatorname{Spec} \begin{pmatrix} A_{11} - \gamma & A_{12} \\ -A_{12}^* & A_{22} + \gamma \end{pmatrix} \Leftrightarrow \gamma \in \operatorname{Spec} \begin{pmatrix} A_{11} - \lambda & A_{12} \\ A_{12}^* & -A_{22} + \lambda \end{pmatrix}.$$

Therefore, it follows that for $\lambda \in \mathbb{C} \setminus \mathbb{R}$, eigenvectors $(\mathbf{u}, \mathbf{v})^T$ corresponding to the real eigenvalues of

$$\begin{pmatrix} A_{11} - \lambda & A_{12} \\ A_{12}^* & -A_{22} + \lambda \end{pmatrix}$$

satisfy $\|\mathbf{u}\| = \|\mathbf{v}\|$.

Remark 2.1.5. Consider Lemma 2.1.3. If, in addition, $\|\mathbf{u}\| = \|\mathbf{v}\| = 1$, then we deduce from (2.5) that

$$|\operatorname{Im}(\lambda)| = |\operatorname{Im}\langle A_{12}\mathbf{v}, \mathbf{u} \rangle|.$$

Theorem 2.1.6. *Consider*

$$\mathbf{X}_0 = \begin{pmatrix} A_{11} & A_{12} \\ -A_{12}^* & A_{22} \end{pmatrix},$$

where $A_{11} = A_{11}^*$ satisfies $\text{Spec}(A_{11}) \subseteq [a_1, a_2]$, and $A_{22} = A_{22}^*$ satisfies $\text{Spec}(A_{22}) \subseteq [d_1, d_2]$. Let $\mathbf{X}_0 \mathbf{f} = \lambda \mathbf{f}$ where $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and $\mathbf{f} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}$ such that $\|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 = 2$. Then

$$\|\mathbf{u}\| = \|\mathbf{v}\| = 1, \tag{2.6}$$

and

$$\max(a_1, d_1) - \delta \leq \text{Re}(\lambda) \leq \min(a_2, d_2) + \delta,$$

where $\delta = |\langle A_{12} \mathbf{v}, \mathbf{u} \rangle|$.

Proof. Equation (2.6) immediately follows from Lemma 2.1.3. Now, re-writing $\mathbf{X}_0 \mathbf{f} = \lambda \mathbf{f}$ in the form

$$\begin{aligned} A_{11} \mathbf{u} + A_{12} \mathbf{v} &= \lambda \mathbf{u}, \\ -A_{12}^* \mathbf{u} + A_{22} \mathbf{v} &= \lambda \mathbf{v}, \end{aligned}$$

leads to

$$\langle A_{11} \mathbf{u}, \mathbf{u} \rangle + \langle A_{12} \mathbf{v}, \mathbf{u} \rangle = \lambda, \tag{2.7}$$

$$-\langle A_{12}^* \mathbf{u}, \mathbf{v} \rangle + \langle A_{22} \mathbf{v}, \mathbf{v} \rangle = \lambda. \tag{2.8}$$

This may be re-written in the form

$$\begin{pmatrix} a & b \\ -\bar{b} & d \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \lambda \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

where $a = \langle A_{11} \mathbf{u}, \mathbf{u} \rangle$, $b = \langle A_{12} \mathbf{v}, \mathbf{u} \rangle$, $\delta = |b|$, and $d = \langle A_{22} \mathbf{v}, \mathbf{v} \rangle$. The theorem now follows directly from Lemma 2.1.1 and the inclusion $a \in [a_1, a_2]$ and $d \in [d_1, d_2]$. \square

Remark 2.1.7. Theorem 2.1.6 is similar to Proposition 1.3.9 from [75] where she estimates

$$\text{Spec}(\mathbf{X}_0) \cap \mathbb{R} \subset [\min(a_1, d_1), \max(a_2, d_2)].$$

Our result is somewhat stronger if $\delta = |\langle A_{12} \mathbf{v}, \mathbf{u} \rangle|$ is small.

2.2 Gershgorin circles

One of the most famous methods which can be used for eigenvalue localisation regions was introduced by the mathematician Semyon Aranovich Gershgorin in 1931 [25]. He observed that the spectrum of a complex matrix is contained in a union of disks in the complex plane, which are nowadays called Gershgorin disks. These disks are centred at the diagonal entries of the matrix and their radii are the row (or column) sum of the moduli of non-diagonal entries; see Theorem 1.3.1 for the formal statement of Gershgorin's result. It is an easy tool to obtain bounds on the eigenvalues without assuming any condition on a matrix. It has many applications, for example, in stability theory (see [68]), in locating the roots of polynomials (see [1, 50, 54, 55]) and controller design (see [32, 64]).

In general, eigenvalue inclusion regions are useful in eigenvalue perturbation theory (see [71, 81]) and in the computation of pseudospectra (see [72]). A good survey of eigenvalue bounds including their rich and interesting history can be found in [31, Chapter 6], whereas [79] provides more advanced and comprehensive results. In this section, the well-known results about Gershgorin-type eigenvalue localizations will be reviewed.

2.2.1 Inclusion regions for the eigenvalues of matrices

We begin by recalling some notation. The (i, j) -th element of the matrix A is denoted by $a_{i,j}$, i.e. $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$. $r_i(A)$ denotes the i -th deleted absolute row sum of A , i.e.

$$r_i(A) := \sum_{j \in J_i} |a_{i,j}|,$$

where $J_i = \{1, 2, \dots, n\} \setminus \{i\}$. We now give a proof of Gershgorin Theorem (Theorem 1.3.1).

Proof of Theorem 1.3.1. Let λ be an eigenvalue of A and \mathbf{x} be a corresponding eigenvector. Suppose the i -th component of \mathbf{x} has the largest modulus; i.e. $|x_i| = \max_j |x_j|$. Looking at the i -th coordinate of the equation $A\mathbf{x} = \lambda\mathbf{x}$, it can be seen that

$$\sum_{j=1}^n a_{i,j}x_j = \lambda x_i \quad \Leftrightarrow \quad a_{i,i}x_i + \sum_{j \in J_i} a_{i,j}x_j = \lambda x_i \quad \Leftrightarrow \quad \sum_{j \in J_i} a_{i,j}x_j = (\lambda - a_{i,i})x_i.$$

Taking the modulus on the both sides of the last equation and applying the triangle inequality and then the maximal property of $|x_i|$ yields

$$|\lambda - a_{i,i}||x_i| = \left| \sum_{j \in J_i} a_{i,j}x_j \right| \leq \sum_{j \in J_i} |a_{i,j}||x_j| \leq |x_i| \sum_{j \in J_i} |a_{i,j}| = |x_i|r_i(A).$$

Since $|x_i| > 0$, dividing both sides of the inequality by $|x_i|$ gives $|\lambda - a_{i,i}| \leq r_i(A)$, i.e. λ lies in a disk with centre $a_{i,i}$ and radius $r_i(A)$. Since it is not clear which i each eigenvalue corresponds to, one needs to take the union of all such disks in order to obtain a guaranteed region. \square

The set $\mathcal{G}_i(A)$ is called the i -th Gershgorin disk of A , which is a closed disk in the complex plane \mathbb{C} , centred at $a_{i,i}$ with a radius of $r_i(A)$. Then $\mathcal{G}(A)$ is the union of the n Gershgorin disk, and it is called the Gershgorin set which is closed and bounded in \mathbb{C} .

Remark 2.2.1. Since the spectra of A and its transpose A^T are identical, an analogous statement is obtained by considering the matrix A^T , with deleted column sums replacing deleted row sums. This will also be true for all the other results in this section unless stated otherwise.

The next well-known result is given by Brauer (1947).

Theorem 2.2.2 ([79, Theorem 2.2]). *Let $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$, $n \geq 2$. Then*

$$\text{Spec}(A) \subseteq \mathcal{K}(A) := \bigcup_{\substack{i,j=1 \\ i \neq j}}^n \mathcal{K}_{i,j}(A),$$

where

$$\mathcal{K}_{i,j}(A) := \{\zeta \in \mathbb{C} : |\zeta - a_{i,i}| |\zeta - a_{j,j}| \leq r_i(A) r_j(A)\}. \quad (2.9)$$

Cassini ovals are a family of quartic curves defined as the set of points such that the product of the distances to two fixed points is constant, and the fixed points are called the foci of the Cassini oval. $\mathcal{K}_{i,j}(A)$ is called the (i, j) -th Brauer Cassini oval for the matrix A , whereas $\mathcal{K}(A)$ is called the Brauer set.

Remark 2.2.3. Note that $\mathcal{G}_i(A)$ is sometimes also called the i -th Gershgorin circle of A . Both (i, j) -th Brauer Cassini oval $\mathcal{K}_{i,j}(A)$ and i -th Gershgorin circle $\mathcal{G}_i(A)$ were named with the shape of their boundaries, however both $\mathcal{K}_{i,j}(A)$ and $\mathcal{G}_i(A)$ are regions bounded by a Cassini oval and a circle respectively.

Remark 2.2.4. For an $n \times n$ matrix, there are $n(n - 1)/2$ ovals of Brauer Cassini, while there are n Gershgorin disks.

The next result is due to Fan and Hoffman (1954).

Theorem 2.2.5 ([79, Theorem 1.20]). *For any matrix $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$, if α is any positive number satisfying ¹*

$$\sum_{i=1}^n \frac{r_i(A)}{\max_{j \in J_i} |a_{i,j}|} \leq \alpha(1 + \alpha),$$

then

$$\text{Spec}(A) \subseteq \bigcup_{i=1}^n \{\zeta \in \mathbb{C} : |\zeta - a_{i,i}| \leq \rho_i\},$$

where

$$\rho_i = \alpha \max_{j \in J_i} |a_{i,j}|. \quad (2.10)$$

Melman found new eigenvalue inclusion sets for matrices without assuming any structure in [50, 52, 55], for structured matrices in [49], and for Toeplitz type matrices in [53], however we shall mention only two of them. Before stating the results, we introduce additional notation. Let $J_{i,j} = \{1, \dots, n\} \setminus \{i, j\}$, then define

$$\tilde{r}_{i,j} := \sum_{k \in J_{i,j}} |a_{i,k}| = r_i - |a_{i,j}| = \sum_{k=1}^n |a_{i,k}| - |a_{i,i}| - |a_{i,j}| \quad (\text{for } i \neq j). \quad (2.11)$$

Theorem 2.2.6 ([50, Theorem 2.1]). *Let $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$. Then*

$$\text{Spec}(A) \subseteq \Omega(A) := \bigcup_{i=1}^n \left\{ \bigcap_{j \in \tilde{J}_i} \Omega_{i,j}(A) \right\},$$

where \tilde{J}_i is any non-empty subset of J_i and

$$\Omega_{i,j}(A) := \{\zeta \in \mathbb{C} : |(\zeta - a_{i,i})(\zeta - a_{j,j}) - a_{i,j}a_{j,i}| \leq |\zeta - a_{j,j}|\tilde{r}_{i,j}(A) + |a_{i,j}|\tilde{r}_{j,i}(A)\}. \quad (2.12)$$

In addition,

$$\Omega_{i,j}(A) \subseteq \mathcal{G}_i(A) \cup \mathcal{G}_j(A) \quad \text{for all } i \neq j.$$

Recall that the matrix is centrohermitian if it is symmetric with respect to its centre, i.e. its elements satisfy $a_{i,j} = \bar{a}_{n-i+1, n-j+1}$, and it is skew-centrohermitian if $a_{i,j} = -\bar{a}_{n-i+1, n-j+1}$, where $\bar{a}_{i,j}$ is the complex conjugate of $a_{i,j}$.

Theorem 2.2.7 ([49, Theorem 2.6]). *Let $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$ such that n is even and A is skew-centrohermitian. Then*

$$\text{Spec}(A) \subseteq \bigcup_{i=1}^n \mathcal{V}_i(A),$$

where $\mathcal{V}_i(A)$ is defined to be the set

$$\{\zeta \in \mathbb{C} : |(\zeta - a_{i,i})(\zeta - \bar{a}_{i,i}) - |a_{i, n-i+1}|^2| \leq (|\zeta + \bar{a}_{i,i}| + |a_{i, n-i+1}|)\tilde{r}_{i, n-i+1}(A)\}. \quad (2.13)$$

¹If $\max_{j \in J_i} |a_{i,j}| = 0 = r_i(A)$ for some i , then $r_i(A)/\max_{j \in J_i} |a_{i,j}|$ is defined to be zero.

2.2.2 Exclusion regions for the eigenvalues of matrices

There are some proper subsets of the Gershgorin set which do not contain any eigenvalue of the matrix. These sets give substantial improvements to determine the location of the eigenvalues of a matrix (cf. [44, 51]). Melman [51] gave the following Gershgorin-type set.

Theorem 2.2.8. *Let $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$. Then*

$$\text{Spec}(A) \subseteq \tilde{\Omega}(A) = \bigcup_{i=1}^n \tilde{\Omega}_i(A),$$

where

$$\tilde{\Omega}_i(A) := \mathcal{G}_i(A) \setminus \mathcal{L}_i(A), \quad \mathcal{L}_i(A) := \bigcup_{j \in J_i} \mathcal{L}_{i,j}(A), \quad (2.14)$$

and

$$\mathcal{L}_{i,j}(A) := \{\zeta \in \mathbb{C} : |\zeta - a_{j,j}| < 2|a_{j,i}| - r_j(A)\}. \quad (2.15)$$

Furthermore, $\tilde{\Omega}(A) \subseteq \mathcal{G}(A)$.

Remark 2.2.9. In [51], there was a typographical error in the definition of $\mathcal{L}_{i,j}(A)$, “ \geq ” instead of “ $<$ ”. What we state here is the corrected version by Li et al. [44].

According to Melman, this result was based on a previous result obtained by Parodi and Schneider. We refer to [79, p.73-79] for detailed discussion of the Parodi and Schneider results. The next result is given by Li et al. [44] in which they gave two new Brauer-type sets. We mention only one of them.

Theorem 2.2.10 ([44, Theorem 4]). *Let $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$. Then*

$$\text{Spec}(A) \subseteq \tilde{\Phi}(A) = \bigcup_{\substack{i,j=1 \\ i \neq j}}^n \tilde{\Phi}_{i,j}(A),$$

where

$$\tilde{\Phi}_{i,j}(A) = \mathcal{K}_{i,j}(A) \setminus \tilde{\mathcal{L}}_i(A), \quad \tilde{\mathcal{L}}_i(A) = \bigcup_{s \in J_i} \tilde{\mathcal{L}}_{s,i}(A), \quad (2.16)$$

and

$$\tilde{\mathcal{L}}_{s,i}(A) = \{\zeta \in \mathbb{C} : |\zeta - a_{s,s}|(|\zeta - a_{i,i}| + \tilde{r}_{i,s}(A)) < (|a_{s,i}| - \tilde{r}_{s,i}(A))|a_{i,s}|\}. \quad (2.17)$$

Furthermore, $\tilde{\Phi}(A) \subseteq \mathcal{B}(A)$.

Remark 2.2.11. It was pointed out in [44] that there are $3n(n-1)/2$ Cassini ovals in the set $\tilde{\Phi}(A)$, whereas $n(n-1)/2$ ones in the set $\mathcal{K}(A)$. Although $\tilde{\Phi}(A)$ usually gives a better bound than the Brauer set $\mathcal{K}(A)$, it takes more time to compute.

2.2.3 Inclusion regions for the eigenvalues of a linear pencil

The first Gerhgorin-type inclusion region for a generalised eigenvalue problem $A\mathbf{x} = \lambda D\mathbf{x}$ appeared in the paper by Stewart and Sun [70, 71]. Let $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$ and $D = [d_{i,j}] \in \mathbb{C}^{n \times n}$.

Theorem 2.2.12. [71, Theorem 2.4] *Let (A, D) be a regular matrix pair, i.e. $\det(A - \lambda D)$ does not vanish identically. Let*

$$\mathcal{S}_i(A, D) = \{\zeta \in \mathbb{C} : |a_{i,i} - \zeta d_{i,i}| \leq \sum_{j \in J_i} |a_{i,j} - \zeta d_{i,j}|\}, \quad i = 1, \dots, n. \quad (2.18)$$

Then

$$\text{Spec}(A - \lambda D) \subset \bigcup_{i=1}^n \mathcal{S}_i(A, D).$$

Note that ζ appears on both sides of the inequality in the sets \mathcal{S}_i so that it may be difficult to compute \mathcal{S}_i in some cases. Therefore, Stewart and Sun [71] gave an alternative bound as follows.

Theorem 2.2.13. [71, Corollary 2.5] *Let \mathcal{X} denote the chordal metric defined by*

$$\mathcal{X}(x, y) = \frac{|x - y|}{\sqrt{1 + |x|^2} \sqrt{1 + |y|^2}}. \quad (2.19)$$

Let

$$\tilde{\mathcal{S}}_i(A, D) \equiv \{\zeta \in \mathbb{C} : \mathcal{X}(\zeta, a_{ii}/d_{ii}) \leq \varrho_i\}, \quad (2.20)$$

where

$$\varrho_i = \sqrt{\frac{\left(\sum_{j \in J_i} |a_{i,j}|\right)^2 + \left(\sum_{j \in J_i} |d_{i,j}|\right)^2}{|a_{i,i}|^2 + |d_{i,i}|^2}}. \quad (2.21)$$

Then

$$\mathcal{S}_i \subset \tilde{\mathcal{S}}_i, \quad i = 1, \dots, n,$$

so that

$$\text{Spec}(A - \lambda D) \subset \bigcup_{i=1}^n \tilde{\mathcal{S}}_i(A, D).$$

2.2.4 Minimal Gershgorin sets

In this section, we review the minimal Gershgorin set which was introduced by Varga in [78]. Its theoretical properties were studied in more detail in [79] and the algorithms for computing the set were developed in [38, 80].

Let $\mathbf{x} = (x_1, \dots, x_n)^T \in \mathbb{R}^n$ be any vector with positive components (which we write as $\mathbf{x} > 0$), and set

$$X := \text{diag}(x_1, \dots, x_n),$$

so that X is non-singular. It is clear that if $A = [a_{i,j}] \in \mathbb{C}^{n \times n}$ then

$$X^{-1}AX = \left[a_{i,j} \frac{x_j}{x_i} \right].$$

Since $\text{Spec}(A) \equiv \text{Spec}(X^{-1}AX)$, applying the Gershgorin's result (i.e. Theorem 1.3.1) to $X^{-1}AX$ gives that i -th Gershgorin disk for $X^{-1}AX$ is given by

$$\mathcal{G}_i^{r_{\mathbf{x}}}(A) := \{ \zeta \in \mathbb{C} : |\zeta - a_{i,i}| \leq r_{\mathbf{x},i}(A) \}, \quad (2.22)$$

where $r_{\mathbf{x},i}(A)$ is the i -th deleted absolute row sum of $X^{-1}AX$, i.e.

$$r_{\mathbf{x},i}(A) := r_i(X^{-1}AX) = \frac{1}{x_i} \sum_{j \in J_i} |a_{i,j}| x_j. \quad (2.23)$$

Then the associated Gershgorin set is given by

$$\mathcal{G}^{r_{\mathbf{x}}}(A) := \bigcup_{i=1}^n \mathcal{G}_i^{r_{\mathbf{x}}}(A),$$

and therefore

$$\text{Spec}(A) \subseteq \mathcal{G}^{r_{\mathbf{x}}}(A).$$

Since this inclusion holds for any $\mathbf{x} > 0$ in \mathbb{R}^n , by intersecting over all $\mathbf{x} > 0$ in \mathbb{R}^n , we obtain

$$\text{Spec}(A) \subseteq \mathcal{G}^{\mathcal{R}}(A) := \bigcap_{\mathbf{x} > 0} \mathcal{G}^{r_{\mathbf{x}}}(A). \quad (2.24)$$

The set $\mathcal{G}^{\mathcal{R}}(A)$ is called the minimal Gershgorin set for A , relative to the collection of all row sums $r_{\mathbf{x},i}(A)$, where $\mathbf{x} > 0$ in \mathbb{R}^n .

In other words, for any nonsingular matrix X , the spectrum of A and $X^{-1}AX$ are the same whereas their Gershgorin sets are not, and one may obtain better estimates by considering the minimal Gershgorin set of a matrix. Indeed, the minimal Gershgorin set gives the sharpest localisation of the spectrum of a matrix among all Gershgorin-type sets

(cf. [37]). Nevertheless, calculating this set for a given matrix is not easy. Therefore, Varga et al. [80] and Kostic et al. [38] proposed numerical algorithms for finding an approximation set, however the applicability of these algorithms are limited to the small or medium size matrices.

2.2.5 Gershgorin sets for block matrices

Gershgorin's theorem was extended to a more general setting of partitioned matrices by Feingold and Varga [23, 79] and to finite matrices of bounded operators on Banach spaces by Salas [65]. The results in this section have more general forms which are applicable to bounded and/or infinite dimensional operators but we will be working on the block matrix \mathbf{X} given in (2.2).

It is well-known (see [26, p. 84]) that the norm of the resolvent of a normal operator can be calculated in terms of the distance to the spectrum, i.e. if A is a normal operator, then

$$\left(\|(\zeta I - A)^{-1}\|\right)^{-1} = \text{dist}(\zeta, \text{Spec}(A)) = \inf_{\lambda \in \text{Spec}(A)} |\zeta - \lambda|, \quad (2.25)$$

where $\zeta \in \mathbb{C} \setminus \text{Spec}(A)$.

The next result is the Gershgorin theorem for the block matrix \mathbf{X} , which is given by Tretter [75].

Theorem 2.2.14. [75, Theorem 1.13.1 and Remark 1.13.4] *Let $A_{11} = A_{11}^*$, $A_{22} = A_{22}^*$ and suppose that $A_{21} = -A_{12}^*$. Then*

(i) *It follows that*

$$\text{Spec}(\mathbf{X}) \subset \{\zeta \in \mathbb{C} : \text{dist}(\zeta, \text{Spec}(A_{11}) \cup \text{Spec}(A_{22})) \leq \|A_{12}\|\}.$$

(ii) *In addition, let*

$$\begin{aligned} \min(\text{Spec}(A_{11})) &= a_-, & \max(\text{Spec}(A_{11})) &= a_+, \\ \min(\text{Spec}(A_{22})) &= d_-, & \max(\text{Spec}(A_{22})) &= d_+. \end{aligned}$$

Then

$$\text{Re}(\text{Spec}(\mathbf{X})) \subset [\min\{a_-, d_-\}, \max\{a_+, d_+\}].$$

There are similar generalisations of the Gershgorin-type results in the block matrix case, see [23, 79]. We mention only Brauer's result on Cassini ovals which was given by Feingold and Varga [23] as the following.

Theorem 2.2.15. [23, Theorem 6] Let $A_{11} = A_{11}^*$, $A_{22} = A_{22}^*$ and suppose that either $A_{21} = A_{12}^*$ or $A_{21} = -A_{12}^*$. Then

$$\text{Spec}(\mathbf{X}) \subset \left\{ \lambda \in \mathbb{C} : \left(\inf_{\zeta \in \text{Spec}(A_{11})} |\lambda - \zeta| \right) \left(\inf_{\zeta \in \text{Spec}(A_{22})} |\lambda - \zeta| \right) \leq \|A_{12}\|^2 \right\}. \quad (2.26)$$

2.2.6 A Gershgorin-type result for the spectrum of a two-parameter eigenvalue problem

In Section 3.2, the general concept of the two-parameter eigenvalue problem will be investigated in more details. In here, we briefly introduce the problem and then we give the Gershgorin-type localisation for the problem. A two-parameter eigenvalue problem is

$$\mathbf{M}(\alpha, \beta) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} A - \alpha & C \\ C^* & D - \beta \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}, \quad (2.27)$$

where A, D are self-adjoint operators in the Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$, respectively, and C is a linear operator from \mathcal{H}_2 to \mathcal{H}_1 . We say that (α, β) is a pair-eigenvalue of \mathbf{M} if there exist a non-zero element $(\mathbf{u}, \mathbf{v})^T \in \mathcal{H}_1 \oplus \mathcal{H}_2$ satisfying (2.27). The set of all pair-eigenvalues of \mathbf{M} will be denoted by $\text{Spec}_p(\mathbf{M})$. The following result is the Gershgorin-type set for the two-parameter eigenvalue problem obtained by applying to Theorem 2.2.15.

Corollary 2.2.16. For the set of pair-eigenvalues of \mathbf{M} defined by (2.27) we have

$$\text{Spec}_p(\mathbf{M}) \subset \mathcal{M}(A, D),$$

where

$$\mathcal{M}(A, D) := \{(\alpha, \beta) \in \mathbb{C}^2 : \text{dist}(\alpha, \text{Spec}(A)) \text{dist}(\beta, \text{Spec}(D)) \leq \|C\|^2\}.$$

Proof of Corollary 2.2.16. Recall the relation between the two-parameter eigenvalue problem (2.27) and the non-self-adjoint problem (1.13). Applying Theorem 2.2.15 to the non-self-adjoint problem (1.13), the set on the RHS of (2.26) becomes

$$\{\lambda \in \mathbb{C} : \text{dist}(\lambda, \text{Spec}(A + c)) \text{dist}(\lambda, \text{Spec}(-D - c)) \leq \|C\|^2\}.$$

Re-arranging the distance function with account of (1.14) gives

$$\text{dist}(\lambda, \text{Spec}(A + c)) = \text{dist}(\lambda - c, \text{Spec}(A)) = \text{dist}(\alpha, \text{Spec}(A)),$$

and similarly

$$\text{dist}(\lambda, \text{Spec}(-D - c)) = \text{dist}(-\lambda - c, \text{Spec}(D)) = \text{dist}(\beta, \text{Spec}(D)).$$

Hence the statement of the corollary follows. □

2.3 Orthogonal polynomials

Let η be a positive Borel measure with support \mathcal{I} defined on \mathbb{R} for which all the moments

$$\eta_k = \int_{\mathcal{I}} x^k d\eta(x), \quad k = 0, 1, 2, \dots,$$

are finite. Let $P_n(x)$ be a polynomial of degree n . Then a sequence of polynomials $\{P_n(x)\}_{n=0}^{\infty}$ is orthogonal with respect to η on \mathcal{I} if

$$\langle P_n, P_m \rangle_{\eta} = \int_{\mathcal{I}} P_n(x)P_m(x)d\eta(x) = h_n\delta_{mn}, \quad m, n = 0, 1, 2, \dots,$$

where δ_{mn} is the Kronecker delta and h_n is the square of the weighted L^2 -norm of P_n given by

$$h_n := \langle P_n, P_n \rangle_{\eta} = \|P_n\|_{\eta}^2 = \int_{\mathcal{I}} (P_n)^2 d\eta(x) > 0.$$

Let $\omega(x)$ denote a weight function which is continuous and positive on (a, b) . Assume the measure η is absolutely continuous with respect to Lebesgue measure and $d\eta(x) = \omega(x)dx$ on some interval (a, b) , then $\{P_n(x)\}_{n=0}^{\infty}$ is called orthogonal on (a, b) with respect to the positive weight function $\omega(x)$ if

$$\langle P_n, P_m \rangle_{\omega} = \int_a^b P_n(x)P_m(x)\omega(x)dx = h_n\delta_{mn}, \quad m, n = 0, 1, 2, \dots$$

If $h_n = 1$ for each $n = 0, 1, 2, \dots$, then the sequence of polynomials is called orthonormal. If $P_n(x) - x^n$ has a degree of at most $n - 1$, then the sequence of polynomials is said to be monic.

Orthogonal polynomials satisfy the three-term recurrence relations that show their relations with continued fractions.

Theorem 2.3.1. [77, Theorem 2.1] *Orthogonal polynomials $P_n(x) = \gamma_n x^n + k_n x^{n-1} + \dots$ on the real line satisfy a three-term recurrence relation*

$$xP_n(x) = a_{n+1}P_{n+1}(x) + b_nP_n(x) + a_nP_{n-1}(x), \quad (2.28)$$

with initial conditions $P_{-1} = 0$ and $P_0 = 1$. The recurrence coefficients are given by

$$a_n = \int xP_{n-1}(x)P(x)d\eta(x) = \frac{\gamma_{n-1}}{\gamma_n} > 0,$$

$$b_n = \int xP_n^2(x)d\eta(x) = \frac{k_n}{\gamma_n} - \frac{k_{n+1}}{\gamma_{n+1}}.$$

See [77] for proof of Theorem 2.3.1.

The orthogonal polynomials are closely related to the Jacobi matrices (or Jacobi operators). These matrices are real, symmetric, tridiagonal matrices with positive off-diagonal entries, and given by

$$\mathcal{J}_n = \begin{pmatrix} b_1 & a_1 & & & \\ a_1 & b_2 & a_2 & & \\ & a_2 & b_3 & \ddots & \\ & & \ddots & \ddots & a_{n-1} \\ & & & a_{n-1} & b_n \end{pmatrix}, \quad a_j > 0, \quad b_j \in \mathbb{R}. \quad (2.29)$$

The Jacobi matrix \mathcal{J}_n has n real distinct eigenvalues and the monic polynomial $P_n(x)/\gamma_n$ is the characteristic polynomial of \mathcal{J}_n . In other words, zeros of P_n are the eigenvalues of \mathcal{J}_n .

2.3.1 Properties of the Chebyshev polynomials of the second kind

Chebyshev polynomials are special cases of the Jacobi polynomials, which are a class of classical orthogonal polynomials. We shall focus our attention only on Chebyshev polynomials of the second kind, denoted by $U_n(x)$. The sequence of polynomials $\{U_n(x)\}_{n=0}^{\infty}$ was first studied by the mathematician P. L. Chebyshev (1821-1894). Formally, they are defined by

$$U_n(x) = \frac{\sin[(n+1)\theta]}{\sin \theta}, \quad \text{when } x = \cos \theta. \quad (2.30)$$

If $x \in [-1, 1]$, then one can take the range of the corresponding variable θ as $[0, \theta]$.

Recall the trigonometric identity

$$\sin[(n+1)\theta] + \sin[(n-1)\theta] = 2 \cos \theta \sin(n\theta). \quad (2.31)$$

If we combine the definition (2.30) with (2.31), then it follows that $U_n(x)$ satisfies the recurrence relation:

$$\begin{aligned} U_0(x) &= 1, \\ U_1(x) &= 2x, \\ U_{j+1}(x) &= 2xU_j(x) - U_{j-1}(x), \quad j \geq 2. \end{aligned} \quad (2.32)$$

It can be seen from (2.30) that the θ -zeros in $[0, \pi]$ of $\sin[(n+1)\theta]$ must correspond to the x -zeros in $[-1, 1]$ of $U_n(x)$, i.e.

$$(n+1)\theta = j\pi, \quad j = 1, 2, \dots, n.$$

Proof. If $i \neq j$, then using

$$x = \cos \theta, \quad dx = -\sin \theta d\theta, \quad (2.38)$$

we have

$$\begin{aligned} \langle U_i, U_j \rangle_w &= \int_{-1}^1 U_i(x)U_j(x)(1-x^2)^{1/2}dx, \\ &= \int_{\pi}^0 \frac{\sin[(i+1)\theta]}{\sin \theta} \frac{\sin[(j+1)\theta]}{\sin \theta} (1-\cos^2 \theta)^{1/2}(-\sin \theta)d\theta, \\ &= \frac{1}{2} \int_0^{\pi} (\cos[(i-j)\theta] - \cos[(i+j+2)\theta])d\theta, \\ &= \frac{1}{2} \left[\frac{\sin[(i-j)\theta]}{(i-j)} - \frac{\sin[(i+j+2)\theta]}{(i+j+2)} \right]_0^{\pi} = 0. \end{aligned}$$

If $j = i$, then again by (2.38), we find the normalization which corresponds to $U_j(x)$ as follows:

$$\begin{aligned} \langle U_i, U_i \rangle_w &= \int_{\pi}^0 \frac{\sin^2[(i+1)\theta]}{\sin^2 \theta} \sin \theta(-\sin \theta)d\theta, \\ &= \frac{1}{2} \int_0^{\pi} (1 - \cos[2(i+1)\theta])d\theta, \\ &= \frac{1}{2} \left[\theta - \frac{\sin[2(i+1)\theta]}{[2(i+1)]} \right]_0^{\pi}, \\ &= \frac{\pi}{2}. \end{aligned}$$

□

Corollary 2.3.4. *Similarly, by the change of variables, we can derive the orthonormal system*

$$\left\{ \sqrt{\frac{1}{\pi}} F_n(x) \right\}_{n=0}^{\infty},$$

on $[-2, 2]$ with respect to the weight function $w(x) = (1 - (x/2)^2)^{1/2}$.

It is well-known that if a polynomial has a repeated (double) root, then its derivative has the same root. Therefore, the next result will be useful later for finding the double roots of $U_n(x)$.

Lemma 2.3.5. *For $n > 0$ and $|x| \neq 1$,*

$$\frac{d}{dz} U_n(x) = \frac{(n+2)U_{n-1}(x) - nU_{n+1}(x)}{2(1-x^2)}. \quad (2.39)$$

We omit the proof of Lemma 2.3.5 as it is based on the chain rule and the trigonometric product identity $\sin a \cos b = \frac{1}{2}(\sin(a+b) + \sin(a-b))$. In addition, this lemma is an exercise in Chapter 2.5, problem 15, [48]. See [48] for further properties of Chebyshev polynomials of the second kind.

2.3.2 Extension of Chebyshev polynomials

Using (2.32), the expressions of $U_n(x)$ can be evaluated for any real x , however the transformation $x = \cos\theta$ is not possible outside the interval $[-1, 1]$. If $|x| > 1$, then we may take the alternative transformation $x = \cosh \Theta$ with Θ in the range $[0, \infty)$. One can verify that the same polynomials as sums of powers of x are generated by

$$U_n(x) = \frac{\sinh(n+1)\Theta}{\sinh \Theta}.$$

We extend the Chebyshev polynomials $U_n(x)$ into a polynomial $U_n(\xi)$ of a complex variable ξ by introducing a related complex variable ω such that

$$\xi = \frac{\omega + \omega^{-1}}{2}. \quad (2.40)$$

Let $|\omega| = r$ and suppose that ω moves on a circle of radius r centred at the origin. In the case $r > 1$, we have

$$\begin{aligned} \omega &= r e^{i\theta} = r \cos \theta + i r \sin \theta, \\ \omega^{-1} &= r^{-1} e^{-i\theta} = r^{-1} \cos \theta - i r^{-1} \sin \theta, \end{aligned}$$

and so, from (2.40),

$$\xi = a \cos \theta + i b \sin \theta. \quad (2.41)$$

where

$$a = \frac{1}{2} (r + r^{-1}), \quad b = \frac{1}{2} (r - r^{-1}).$$

Hence the map (2.40) transforms a circle into an ellipse centred at the origin, with major semi-axes a , minor semi-axes b , and with foci at $\xi = \pm 1$.

If $r = 1$, i.e. ω moves on the unit circle, then we obtain $b = 0$ and ellipse collapses into the real interval $[-1, 1]$. However, ξ moves the interval twice as ω travels around the unit circle.

Now, unless z lies on the interval $[-1, 1]$, the equation $\omega + \omega^{-1} = 2\xi$ has two solutions for ω

$$\omega = \omega_{1,2} = \xi \pm \sqrt{\xi^2 - 1}.$$

However, they are inverses of each other. This means that $\omega \mapsto \xi$ is a two-to-one mapping, with branch points at $\xi = \pm 1$. We need to cut the plane along the interval $[-1, 1]$ so as

to define the complex square root $\sqrt{\xi^2 - 1}$ in a way that it lies in the same quadrant as ξ . Therefore, we choose

$$\omega = \omega_1 = \xi + \sqrt{\xi^2 - 1}, \quad (2.42)$$

so that $|\omega| = |\omega_1| \geq 1$ and $|\omega_2| = |\omega_1^{-1}| < 1$. Then ω depends continuously on ξ along any path that does not intersect the interval $[-1, 1]$.

To extend the Chebyshev polynomials of the second kind, we define ξ by (2.40) and assume $|\omega| = r = 1$. We then obtain by (2.41) that

$$\xi = \cos \theta$$

and so, using (2.42),

$$\omega = \xi + \sqrt{\xi^2 - 1} = e^{i\theta},$$

where we fixed a branch of a square root so that $\sqrt{-1} = i$. Hence $U_n(\xi)$ is now a Chebyshev polynomials in a real variable. Then the definition (2.30) gives

$$U_{n-1}(\xi) = \frac{\sin(n\theta)}{\sin \theta} = \frac{\frac{1}{2}(e^{in\theta} - e^{-in\theta})}{\frac{1}{2}(e^{i\theta} - e^{-i\theta})},$$

which leads us to the general definition, for all $\xi \in \mathbb{C}$,

$$U_{n-1}(\xi) = \frac{\omega^n - \omega^{-n}}{\omega - \omega^{-1}} \quad (2.43)$$

where

$$\xi = \frac{1}{2} (\omega + \omega^{-1}).$$

Hence, $U_n(\xi)$ is the analytic continuation of $U_n(x)$ to the complex plane since we extended the values of $U_n(x)$ across a branch cut in the complex plane.

2.3.3 Spectral properties of $H_0^{(n)}$

In this section, we want to construct the basis of eigenfunctions of $H_0^{(n)}$ explicitly. Let $\mu_j^{(n)}$ be the eigenvalues of the matrix H_0 , defined by (2.37), and ψ_j be corresponding eigenvectors, i.e.

$$H_0^{(n)} \psi_j = \mu_j^{(n)} \psi_j, \quad j = 1, 2, \dots, n. \quad (2.44)$$

Lemma 2.3.6. For an arbitrary $n \in \mathbb{N}$, an eigenfunction corresponding to the eigenvalue $\mu_j^{(n)}$ of $H_0^{(n)}$ is

$$\boldsymbol{\psi}_j = \begin{pmatrix} \psi_{j,1} \\ \psi_{j,2} \\ \vdots \\ \psi_{j,n} \end{pmatrix} \quad \text{with} \quad \psi_{j,k} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{\pi j k}{n+1}\right), \quad k = 1, \dots, n. \quad (2.45)$$

Proof. Recall the *Chebyshev method* for finding the n^{th} multiple angle formula for the sine function

$$\sin(n+1)x + \sin(n-1)x = 2 \cos x \sin(nx). \quad (2.46)$$

The equation (2.44) is written in components as

$$\begin{aligned} \psi_{j,2} &= \mu_j \psi_{j,1}, \\ \psi_{j,k-1} + \psi_{j,k+1} &= \mu_j \psi_{j,k}, \quad k = 2, 3, \dots, n-1, \\ \psi_{j,n-1} &= \mu_j \psi_{j,n}. \end{aligned}$$

Substituting (2.45) and (2.37) into above, it can be seen that all n equations hold by (2.46). \square

Note that all eigenvalues of H_0 are simple. If $j \neq k$, then

$$\left. \begin{aligned} \langle H_0 \boldsymbol{\psi}_j, \boldsymbol{\psi}_k \rangle &= \mu_j \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_k \rangle \\ \langle \boldsymbol{\psi}_j, H_0 \boldsymbol{\psi}_k \rangle &= \mu_k \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_k \rangle \end{aligned} \right\} \Rightarrow (\mu_j - \mu_k) \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_k \rangle = 0,$$

which implies that the eigenvector basis $\{\boldsymbol{\psi}_j\}_{j=1}^n$ is orthogonal. Since the matrix $H_0^{(n)}$ is Hermitian, the sequence of eigenfunctions $\{\boldsymbol{\psi}_j\}$ of $H_0^{(n)}$ forms an orthonormal basis by the spectral theorem. Therefore, for a given dimension n , the norm of $\boldsymbol{\psi}_j$ is given by

$$\|\boldsymbol{\psi}_j\|^2 = \frac{2}{n+1} \sum_{k=1}^n \sin^2 \frac{\pi j k}{n+1} = 1, \quad j = 1, \dots, n. \quad (2.47)$$

Remark 2.3.7. One can show (2.47) by using the Dirichlet kernel

$$1 + 2 \sum_{k=1}^n \cos(kx) = \frac{\sin\left[\left(n + \frac{1}{2}\right)x\right]}{\sin\left(\frac{x}{2}\right)}, \quad (2.48)$$

and the trigonometric identity

$$\sin^2\left(\frac{x}{2}\right) = \frac{1 - \cos x}{2}. \quad (2.49)$$

2.3.4 Ratios of Chebyshev polynomials of the second kind

In this section, we state the ratio asymptotics given by B. Simon [66] when applied to the Chebyshev polynomials of the second kind. We will then use these results in a linear pencil problem in Section 4.2.1. Recall that F_n is a monic orthogonal polynomial and the ratio asymptotics we will state is based on the ratio

$$\frac{F_{n+1}(\zeta)}{F_n(\zeta)} = \frac{U_{n+1}(\zeta/2)}{U_n(\zeta/2)}. \quad (2.50)$$

In addition, recall that the zeros of $F_n(\zeta)$ are the eigenvalues of $H_0^{(n)}$ given by (2.37), and $H_0^{(n)}$ is the Jacobi matrix. Simon obtained the following results.

Theorem 2.3.8 ([66, Theorem 2.1]). *For all $\zeta \in \mathbb{C} \setminus [-2, 2]$*

$$\lim_{n \rightarrow \infty} \frac{F_{n+1}(\zeta)}{F_n(\zeta)} = \frac{\zeta + \sqrt{\zeta^2 - 4}}{2}, \quad (2.51)$$

where the branch of the square root is taken with $\sqrt{\cdot} = \zeta + O(1/\zeta)$ near $\zeta = \infty$.

Theorem 2.3.9 ([66, Theorem 2.2]). *Suppose that for one ζ_0 with $\text{Im}(\zeta_0) \neq 0$,*

$$\lim_{n \rightarrow \infty} \frac{F_{n+1}(\zeta)}{F_n(\zeta)}$$

exists and is finite. Then the only function that can occur as ratio asymptotics is the one in (2.51).

Proposition 2.3.10 ([66, Proposition 2.3]).

(i)

$$\frac{F_{n-1}(\zeta)}{F_n(\zeta)} = \sum_{j=1}^n \frac{a_j^{(n)}}{\zeta - \mu_j^{(n)}}, \quad (2.52)$$

where $\alpha_j^{(n)} > 0$ and

$$\sum_{j=1}^n a_j^{(n)} = 1. \quad (2.53)$$

(ii) *If $\text{Im}\zeta > 0$, then*

$$0 < -\text{Im} \left(\frac{F_{n-1}(\zeta)}{F_n(\zeta)} \right) \leq \frac{1}{\text{Im}\zeta} \quad (2.54)$$

and

$$\left| \frac{F_{n-1}(\zeta)}{F_n(\zeta)} \right| \leq \frac{1}{\text{Im}\zeta}.$$

(iii) If $\text{Im}\zeta > 0$, then

$$\text{Im}(\zeta) \leq \text{Im} \left(\frac{F_n(\zeta)}{F_{n-1}(\zeta)} \right).$$

Proof. (i) Since F_n is monic, the ratio can be written as

$$\frac{F_{n-1}(\zeta)}{F_n(\zeta)} = \frac{\prod_{k=1}^{n-1} (\zeta - \mu_k^{(n-1)})}{\prod_{j=1}^n (\zeta - \mu_j^{(n)})}. \quad (2.55)$$

Since $F_n(\zeta)/F_{n-1}(\zeta)$ has simple poles and tends to zero at infinity, equation (2.52) holds for some $\alpha_j^{(n)}$. Multiplying equation (2.52) by $\zeta - \mu_i^{(n)}$ we have

$$\frac{\prod_{k=1}^{n-1} (\zeta - \mu_k^{(n-1)})}{\prod_{\substack{j=1 \\ j \neq i}}^n (\zeta - \mu_j^{(n)})} = \alpha_i^{(n)} + \left(\sum_{\substack{j=1 \\ j \neq i}}^n \frac{\alpha_j^{(n)}}{\zeta - \mu_j^{(n)}} \right) (\zeta - \mu_i^{(n)}).$$

Then taking ζ to $\mu_i^{(n)}$, we obtain

$$\alpha_i^{(n)} = \frac{\prod_{k=1}^{n-1} (\mu_i^{(n)} - \mu_k^{(n-1)})}{\prod_{\substack{j=1 \\ j \neq i}}^n (\mu_i^{(n)} - \mu_j^{(n)})}. \quad (2.56)$$

Note that for any $j = 1, \dots, n-1$

$$\mu_j^{(n)} < \mu_j^{(n-1)} < \mu_{j+1}^{(n)}.$$

Therefore for $i = n$, all factors on the right hand side of (2.56) are positive, and when we decrease i by one, both numerator and denominator each pick up a minus sign. Hence $\alpha_i^{(n)} > 0$. As $\zeta \rightarrow \infty$, it can be seen from (2.55) that the ratio equals to $\zeta^{-1} + O(\zeta^{-2})$. Also from the right side of (2.52) we have that

$$\zeta^{-1} \left(\sum_{j=1}^n \alpha_j^{(n)} \right) + O(\zeta^{-2}),$$

so (2.53) holds.

(ii) First, note that for any $b \in \mathbb{R}$ and $\zeta \in \mathbb{C}$ with $\text{Im}(\zeta) > 0$

$$0 < \text{Im} \left(\frac{1}{\zeta - b} \right) \leq \left| \frac{1}{\zeta - b} \right| \leq \frac{1}{\text{Im}(\zeta)}.$$

Then using (2.52) we obtain

$$\text{Im} \left(\frac{F_{n-1}(\zeta)}{F_n(\zeta)} \right) = \text{Im} \left(\sum_{j=1}^n \frac{a_j^{(n)}}{\zeta - \mu_j^{(n)}} \right) \leq \sum_{j=1}^n \frac{a_j^{(n)}}{\text{Im}(\zeta)} = \frac{1}{\text{Im}(\zeta)}.$$

(iii) Re-write the recurrence relation (2.35) as

$$z = \frac{F_n(\zeta)}{F_{n-1}(\zeta)} + \frac{F_{n-2}(\zeta)}{F_{n-1}(\zeta)}.$$

Since $\text{Im}(F_{n-2}(\zeta)/F_{n-1}(\zeta)) < 0$ by (2.54), the result follows by considering the imaginary parts of the equation. □

The size of both matrices is $N \times N$, and the diagonal matrix $S_{m,n}$ has m plus ones and n minus ones. The number λ_0 is said to be an eigenvalue of the pencil \mathcal{A}_c if

$$(H_c^{(N)} - \lambda S_{m,n}) \mathbf{f} = 0 \quad (3.3)$$

has a non-zero solution $\mathbf{f} \in \mathbb{C}^N$. $\text{Spec}(\mathcal{A}_c)$ denotes the *spectrum* of the pencil \mathcal{A}_c which is the set of all its eigenvalues.

In most of our statements, we assume that $m = n$ and $N = 2n$. We will mostly use 2×2 block structures and so we will often work with the half-size matrix $H_0^{(n)}$. In the notation $H_0^{(n)}$, the superscript (n) represents its size. For simplicity, we often drop the superscript (n) in $H_c^{(n)}$ whenever it is clear from the context, i.e. $H_c := H_c^{(n)}$, and we will state it otherwise. The full matrix size is N and will not be omitted. Recall that the eigenvalues of $H_0^{(n)}$ were denoted by $\mu_j^{(n)}$ in (2.37), and for the same reason, we set $\mu_j := \mu_j^{(n)}$. Moreover, we denote for brevity $S := S_{n,n}$.

We begin with the following result on the localisation of eigenvalues of the pencil \mathcal{A}_c .

Lemma 3.1.1 ([19, Lemma 2.1]). *All the eigenvalues $\lambda \in \text{Spec}(\mathcal{A}_c)$ satisfy*

$$|\lambda| < 2 + |c|.$$

Proof. Note that $\|H_0\| = \mu_1 = 2 \cos(\pi/(N+1)) < 2$. Since $\text{Spec}(\mathcal{A}_c) \equiv \text{Spec}(S^{-1}H_c)$, we have

$$|\lambda| \leq \|S^{-1}H_c\| = \|H_c\| = \|H_0 + cI\| < 2 + |c|.$$

□

The matrix S is indefinite. Since $\text{Spec}(H_c^{(N)}) \equiv \text{Spec}(H_0^{(N)} + cI)$ and $\text{Spec}(H_0^{(N)}) = \{\mu_1^{(N)}, \dots, \mu_N^{(N)}\}$, the matrix $H_c^{(N)}$ is indefinite when $c \in (\mu_N^{(N)}, \mu_1^{(N)}) \subset (-2, 2)$. Therefore, the spectrum $\text{Spec}(\mathcal{A}_c)$ may contain non-real eigenvalues when $|c| < \mu_1^{(N)}$. Davies and Levitin [19] pursued an asymptotic approach for large-size matrices (i.e. $N \rightarrow \infty$) and they obtained the asymptotics of the complex eigenvalues of \mathcal{A}_c when the parameter c is equal to zero. They proved that when $c = 0$ all eigenvalues of \mathcal{A}_c approximately lie on the same curve, which is independent of N , in coordinates $(\text{Re}(\lambda), N\text{Im}(\lambda))$. The curve is explicitly given in the next result.

Theorem 3.1.2 ([19, Theorem 4.2]). *Let $c = 0$, $n = m = N/2 \rightarrow \infty$. The eigenvalues of \mathcal{A}_c are all non-real, and those not lying on the imaginary axis satisfy*

$$\text{Im}(\lambda) = \pm \frac{Y_0(|\text{Re}(\lambda)|)}{2n} + o(n^{-1}),$$

$$\operatorname{Re}(\lambda) = \pm 2 \cos \left(\frac{2\pi k}{2n+1} \right) + o(n^{-1}),$$

where $k = 1, \dots, \lfloor \frac{n}{2} \rfloor$ and $\lfloor \cdot \rfloor$ denotes the integer part, and

$$Y_0(y) := \sqrt{4-y^2} \log \left(\tan \left(\frac{\pi}{4} + \frac{1}{2} \arccos \left(\frac{y}{2} \right) \right) \right).$$

If n is even, then there are no other eigenvalues.

If n is odd, there are additionally two purely imaginary eigenvalues at

$$\lambda = \pm i \frac{\log(n)}{n} (1 + o(1)).$$

We omit numerical illustrations concerning the asymptotics given in Theorem 3.1.2. Instead, we illustrate the eigenvalues of \mathcal{A}_0 for some n in Figure 3.1. For a more detailed discussion on the asymptotics of the complex eigenvalues of \mathcal{A}_0 , we refer the reader to [19].

We will see in most of our numerical experiments that there is symmetry in the spectrum $\operatorname{Spec}(\mathcal{A}_c)$.

Lemma 3.1.3 ([19, Lemma 2.1(a) and Lemma 5.1]). *Let $n = m$. Then the spectrum $\operatorname{Spec}(\mathcal{A}_c)$ is invariant under the symmetry $\lambda \rightarrow \bar{\lambda}$ and the symmetry $\lambda \rightarrow -\lambda$. Moreover $\operatorname{Spec}(\mathcal{A}_c)$ is symmetric with respect to $c \rightarrow -c$.*

Remark 3.1.4. As mentioned above, Davies and Levitin [19] found the approximate locations of the eigenvalues of \mathcal{A}_c when $c = 0$. As the central focus of this study is the case $|c| < 2$ and the spectrum of \mathcal{A}_c is invariant under the symmetry $c \rightarrow -c$, it will be sufficient to consider only the case $0 < c < 2$.

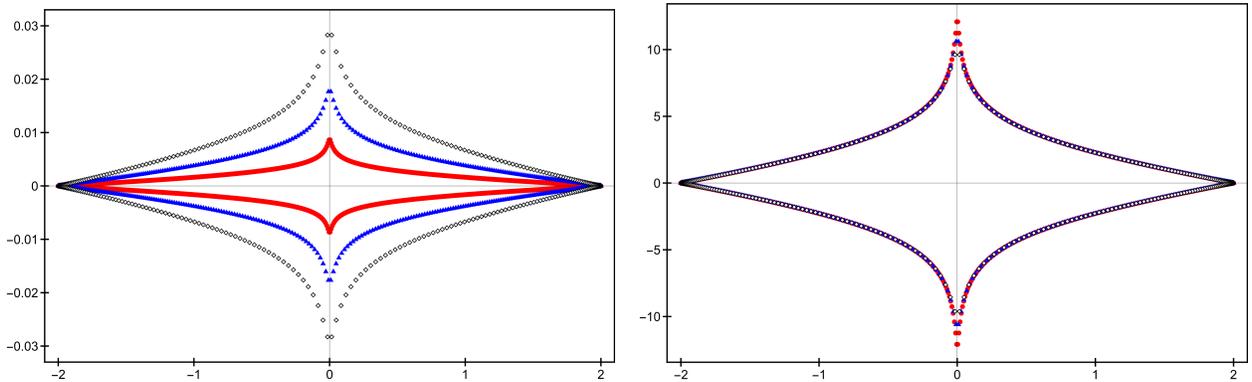


Figure 3.1: $\operatorname{Spec}(\mathcal{A}_0)$ for $n = 170$ (black diamonds), $n = 300$ (blue triangles) and $n = 700$ (red circles). Left: in coordinates $(\operatorname{Re}(\lambda), \operatorname{Im}(\lambda))$. Right: in coordinates $(\operatorname{Re}(\lambda), 2n \operatorname{Im}(\lambda))$.

As can be seen from the left side of Figure 3.1, the spectra asymptotically lie on a particular curve in the complex plane $(\text{Re}(\lambda), \text{Im}(\lambda))$. If one redrew the eigenvalues in coordinates $(\text{Re}(\lambda), N\text{Im}(\lambda))$, one would see that they approximately lie on the same curve, as in the right side of Figure 3.1. Nevertheless, the spectral picture is more complicated when $c \neq 0$ (see the left side of Figure 3.2). The spectrum of \mathcal{A}_c contain both real and non-real eigenvalues and it is hard to believe that the non-real eigenvalues for a fixed c lie on a certain curve.

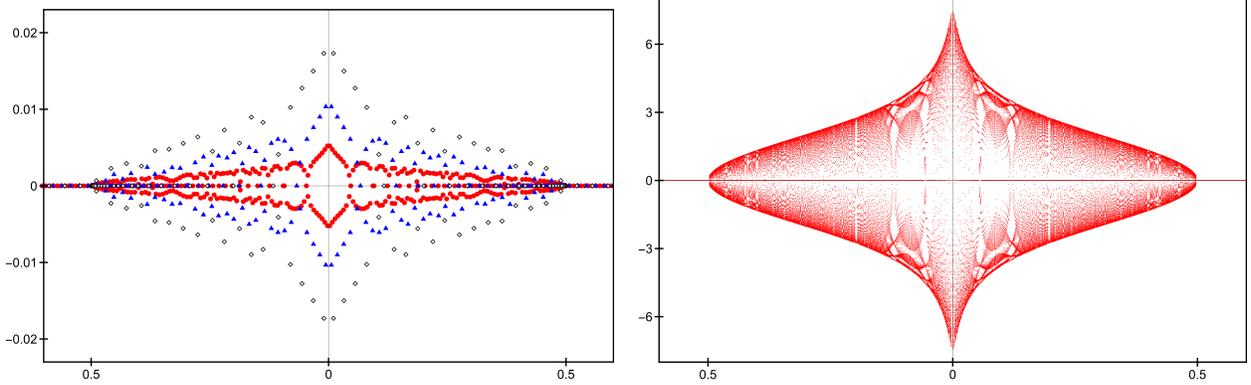


Figure 3.2: Left: $\text{Spec}(\mathcal{A}_c)$ for $c = 1.5$, and $n = 170$ (white diamonds), $n = 300$ (blue triangles) and $n = 700$ (red circles) in coordinates $(\text{Re}(\lambda), \text{Im}(\lambda))$. Right: $\cup_{n=1}^{600} \text{Spec}(\mathcal{A}_c)$ for $c = 1.5$ in coordinates $(\text{Re}(\lambda), 2n\text{Im}(\lambda))$.

Nonetheless, there is a common bounding curve if one superimposes all the eigenvalues of the pencil \mathcal{A}_c by taking some values of n with imaginary parts scaled by its size N (see the right side of Figure 3.2). Note that the behaviour in the interior differs for different c . Davies and Levitin [19] derived an explicit expression for the curve which bounds the whole spectrum of \mathcal{A}_c , however the crucial step when proving the result was Conjecture 1.3.3. Namely, Davies and Levitin [19] deduced the following asymptotic estimates when c is non-zero as $N \rightarrow \infty$.

Theorem 3.1.5 ([19, Theorem 5.4]). *Let $0 < c < 2$, $n = m = N/2 \rightarrow \infty$. The eigenvalues of \mathcal{A}_c that satisfy*

$$|\text{Re}(\lambda)| < 2 - c$$

also satisfy

$$|\text{Im}(\lambda)| \leq \frac{Y_c(|\text{Re}(\lambda)|)}{2n} + o(n^{-1}),$$

where

$$Y_c(y) := \mathcal{Y}_{c,y}^{-1} \left(\tan \left(\frac{1}{2} \arccos \left(\frac{y-c}{2} \right) \right) \tan \left(\frac{1}{2} \arccos \left(\frac{y+c}{2} \right) \right) \right),$$

and $\mathcal{Y}_{c,y}^{-1}$ is the inverse of the monotonic increasing analytic function $\mathcal{Y}_{c,y} : (0, \infty) \rightarrow (0, 1)$ defined by

$$\mathcal{Y}_{c,y}(x) := \tanh\left(\frac{x}{2\sqrt{4 - (y - c)^2}}\right) \tanh\left(\frac{x}{2\sqrt{4 - (y + c)^2}}\right).$$

We shall derive the characteristic polynomial of the pencil \mathcal{A}_c explicitly in Section 4.1.1. Now, we will have a look at some open questions from [19] and try to make some progress towards them. We paid a lot of attention to try to prove Conjecture 1.3.3. Proving (1.16) may be harder than proving (1.17). In Section 4.2 we reformulate the harder modulus version of Conjecture 1.3.3 in different forms. We emphasise that extensive numerics confirm Conjecture 1.3.3. One numerical evidence can be seen, for instance, in Figure 1.2, where we show that the maximum value of $|\lambda \pm c|$ (red line) never exceeds 2 (blue dotted line) for $n = 9$ and $n = 100$. We conducted some experiments taking n between 3 and 300, and taking very small step sizes c , and we failed to find a counter example to the conjecture. In Figure 3.3, we illustrate two typical pictures. We also prove this conjecture in the case $n = 2$ and $n = 3$ in Section 4.3. We will illustrate in various ways with many other numerical experiments that Conjecture 1.3.3 seems true, however we could not prove it for a fixed n .

Conjecture 1.3.3 claims that any non-real eigenvalues λ of the pencil \mathcal{A}_c satisfies both $|\lambda + c| < 2$ and $|\lambda - c| < 2$. First, it is easy to see that two of these conditions cannot be broken simultaneously and we will clarify this case, that is both $|\lambda + c|$ and $|\lambda - c|$ cannot be greater than or equal to 2, in Section 4.2.1. Nevertheless, it is not clear why one of these conditions cannot be broken for the non-real eigenvalues of \mathcal{A}_c . When we apply Gershgorin Theorem to \mathcal{A}_c , we will see in Section 4.2.3 that every eigenvalue of \mathcal{A}_c satisfies at least one of $|\lambda + c| < 2$ and $|\lambda - c| < 2$. Therefore, if we replace "and" by "or" in the conjecture, then the claim would be true by Gershgorin Theorem but then the result holds for all eigenvalues of \mathcal{A}_c .

Remark 3.1.6. There are several ways to treat the pencil problem (3.3). One way is to act by \mathcal{A}_c on vectors which we will write as

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} u_1 \\ \vdots \\ u_n \\ v_n \\ \vdots \\ v_1 \end{pmatrix}. \quad (3.4)$$

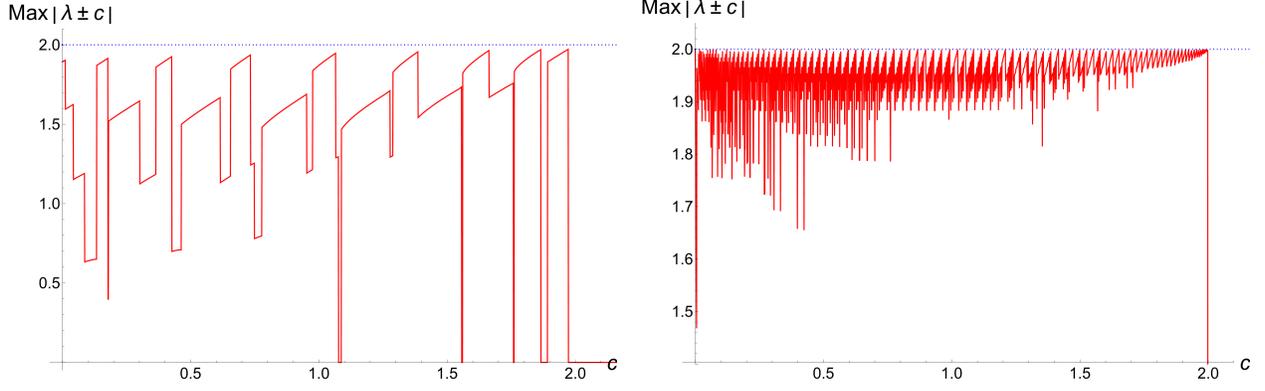


Figure 3.3: $\max\{|\lambda + c|, |\lambda - c|\}$ (red lines) among all non-real eigenvalues of \mathcal{A}_c is drawn as c ranges from 0 to 2 with the step-size 0.001 and the constant line at 2 (blue dotted lines). Left: $n = 9$. Right: $n = 100$.

With this convention, the spectral problem for the linear pencil \mathcal{A}_c can be written in the block-matrix form as

$$\begin{pmatrix} H_0 - \sigma I & B \\ B & H_0 + \tau I \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}, \quad (3.5)$$

where

$$\sigma = \lambda - c; \quad \tau = \lambda + c. \quad (3.6)$$

Here all sub-blocks are $n \times n$, and $B = B^*$ with $B_{nn} = 1$ and all other entries of B are zeros.

Remark 3.1.7. Since S is invertible, the spectrum of the pencil \mathcal{A}_c equals that of the matrix

$$\mathbf{A}_c := S^{-1} H_c^{(N)}. \quad (3.7)$$

Using (3.4), the spectral problem for the block matrix \mathbf{A}_c can be written as

$$\mathbf{A}_c \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} H_c & B \\ -B & -H_c \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}. \quad (3.8)$$

The next result is a special case of Lemma 2.1.3 when $A_{11} = H_0$, $A_{22} = -H_0$, $A_{12} = B$ and $\gamma = -c$.

Corollary 3.1.8. *Let $\lambda \in \text{Spec}(\mathbf{A}_c) \setminus \mathbb{R}$ and $(\mathbf{u}, \mathbf{v})^T$ be eigenvectors which correspond to the non-real eigenvalues λ of \mathbf{A}_c . Then*

$$\|\mathbf{u}\| = \|\mathbf{v}\| \quad \text{and} \quad |\text{Im}(\lambda)| \leq 1.$$

Our original motivation was to try to prove Conjecture 1.3.3 but we could not, nevertheless we still gain some insight and obtain new estimates. The first thing we observed when we considered problem (3.5) in a more general setting, that is,

$$\begin{pmatrix} A - \sigma & \kappa C \\ \kappa C^* & D + \tau \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = 0, \quad (3.9)$$

where $\kappa \in \mathbb{R}$, $A = A^*$, $D = D^*$ and C has rank one. Indeed, problem (3.9) is a special case of a two-parameter eigenvalue problem which we describe in the next section. Namely, Davies and Levitin [19] consider the case when $\kappa = 1$, $A = H_0^{(n)}$, $D = H_0^{(m)}$, $(C)_{n,1} = 1$ and all other entries of C are zeros. In the next section, we shall introduce the general concept of a two-parameter eigenvalue problem first and then explain the relation between eigenvalue problems.

3.2 Introduction to a two-parameter eigenvalue problem

This section deals with the Multiparameter Eigenvalue Problems (MEPs) which are the generalisation of the one-parameter standard eigenvalue problem $L\mathbf{x} = \lambda\mathbf{x}$ and the generalised one-parameter eigenvalue problem $L\mathbf{x} = \lambda V\mathbf{x}$. MEPs can be written in the following abstract form:

$$L\mathbf{x} = \sum_{i=1}^k \lambda_i V_i \mathbf{x}, \quad (3.10)$$

where $\lambda_i \in \mathbb{C}$, $i = 1, 2, \dots, k$, are spectral parameters, and L and V_i are self-adjoint linear operators in some Hilbert space \mathcal{H} . Then $\lambda = (\lambda_1, \dots, \lambda_k)$ is called a *multi-parametric eigenvalue* (or *k-tuple*, or *eigentuple*) if there exists an $\mathbf{x} \in \mathcal{H} \setminus \{0\}$, called an *eigenvector*, such that (3.10) holds.

MEPs arise in numerous applications, in particular in mathematical physics when the method of separation of variables is used to solve boundary value problems for partial differential equations. In the 1960s, an abstract algebraic setting for MEPs was introduced by Atkinson [2, 3], and since then various aspects of MEPs have been investigated by several authors, see for instance [4, 10–12, 67] and references therein.

In the rest of this chapter, we consider a special class of two-parameter eigenvalue problems in a block-operator setting. Let \mathbf{L} , \mathbf{V}_1 and \mathbf{V}_2 be self-adjoint linear operators in some Hilbert space \mathcal{H} . Then a *two-parameter eigenvalue problem* is defined as

$$\mathbf{M}(\alpha, \beta)\mathbf{x} := (\mathbf{L} - \alpha\mathbf{V}_1 - \beta\mathbf{V}_2)\mathbf{x} = 0, \quad (3.11)$$

where $\alpha, \beta \in \mathbb{C}$ are spectral parameters. We will focus on the case where $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ for some Hilbert spaces \mathcal{H}_1 and \mathcal{H}_2 , and where \mathbf{L} , \mathbf{V}_1 and \mathbf{V}_2 take the particular forms

$$\mathbf{L} = \begin{pmatrix} A & C \\ C^* & D \end{pmatrix}, \quad \mathbf{V}_1 = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{V}_2 = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \quad (3.12)$$

and

$$\mathbf{x} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \in \mathcal{H}_1 \oplus \mathcal{H}_2.$$

In here, A and D are self-adjoint operators in the Hilbert spaces \mathcal{H}_1 , \mathcal{H}_2 , respectively, and C is a linear operator from \mathcal{H}_2 to \mathcal{H}_1 . Hence one can re-write the two-parameter eigenvalue problem (3.11) as

$$\mathbf{M}(\alpha, \beta) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} A - \alpha & C \\ C^* & D - \beta \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}. \quad (3.13)$$

We call $(\alpha, \beta) \in \mathbb{C}^2$ a *pair-eigenvalue* of $\mathbf{M} = \mathbf{M}(\alpha, \beta)$ if there exists a non-trivial solution $\mathbf{x} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \in \mathcal{H}$ of (3.13). Such a vector \mathbf{x} is called an *eigenvector* corresponding to the pair-eigenvalue (α, β) . We denote by $\text{Spec}_p(\mathbf{M})$ the set of all pair-eigenvalues of \mathbf{M} . If both $\alpha, \beta \in \mathbb{R}$, then we will call (α, β) a *real pair-eigenvalue* of (3.13).

The equation (3.13) can be re-written as

$$(A - \alpha)\mathbf{u} = -C\mathbf{v}, \quad (3.14)$$

$$(D - \beta)\mathbf{v} = -C^*\mathbf{u}. \quad (3.15)$$

If $\alpha \notin \text{Spec}(A)$, then (3.14) can be re-written as $\mathbf{u} = -(A - \alpha)^{-1}C\mathbf{v}$, and substituting this into (3.15) yields

$$(D - C^*(A - \alpha)^{-1}C)\mathbf{v} = \beta\mathbf{v}. \quad (3.16)$$

This also means that if $\alpha \notin \text{Spec}(A)$ and $\beta(\alpha)$ is an eigenvalue of

$$D - C^*(A - \alpha)^{-1}C,$$

then $(\alpha, \beta(\alpha)) \in \text{Spec}_p(\mathbf{M})$.

The connection between a two-parameter eigenvalue problem (3.13) and a linear pencil problem (1.2) was obtained in Section 1.3 by setting

$$\alpha = \lambda - c; \quad \beta = -\lambda - c. \quad (3.17)$$

With this convention, we see that any linear pencil problem of the form (1.10) (or a non-self-adjoint problem of the form (1.13)) can be transformed into the two-parameter eigenvalue of the form (3.13).

Indeed, it can be said that Davies and Levitin [19] consider the two-parameter eigenvalue problem (3.13) in the case when $A = H_0^{(n)}$, $D = H_0^{(m)}$, $(C)_{n,1} = 1$ and all other entries of C are zeros. In this section, we set (α, β) as general spectral parameters of a two-parameter eigenvalue problem M . In this setting, the corresponding change of notations will be

$$\alpha = \sigma; \quad \beta = -\tau.$$

We shall plot the pair-eigenvalues of M in the (α, β) -plane, whereas σ and τ is fixed as in (3.6) throughout this thesis.

3.3 Basics and statements

In the rest of this chapter, we investigate the real pair-eigenvalues (α, β) of the two-parametric eigenvalue problem (3.13) with starting additional restrictions in Section 3.3.1. We discuss the non-real pair-eigenvalues of M only in Section 3.7. We also give some heuristics for the localisation of the eigenvalues of the pencil \mathcal{A}_c in the aspect of a two parametric eigenvalue problem in Section 5.2.

3.3.1 Restrictions and notation

Suppose that \mathcal{H}_1 and \mathcal{H}_2 are finite dimensional, and therefore we are dealing with matrices. Take $\dim(\mathcal{H}_1) = n$ and $\dim(\mathcal{H}_2) = m$. First, we focus our attention to only the real pair-eigenvalues of M . Our main results (Theorem 3.3.6 and its special case Theorem 3.3.4) are stated below.

Remark 3.3.1. Most of the results in the rest of this chapter have been published in [41]. Note that Levitin and Ozturk [41] deal with the case when $n = m$. What we discuss in here is the expanded version of [41].

Unless otherwise stated, we set

$$i = 1, \dots, n, \quad k = 1, \dots, n-1, \quad j = 1, \dots, m, \quad l = 1, \dots, m-1$$

which will be used as subscripts. The eigenvalues of A and D will be denoted by

$$\alpha_1 \leq \dots \leq \alpha_n, \quad \beta_1 \leq \dots \leq \beta_m,$$

respectively, and their corresponding eigenvectors will be denoted by φ_i and ψ_j , respectively.

In stating most of our results, we restrict our attention to the case where C has rank one. More specifically, we choose two vectors $\mathbf{z} \in \mathbb{R}^n$ and $\mathbf{w} \in \mathbb{R}^m$ (the real one are chosen for simplicity), and set

$$C\mathbf{v} = \kappa \langle \mathbf{v}, \mathbf{w} \rangle \mathbf{z}, \quad \text{for all } \mathbf{v} \in \mathcal{H}_2,$$

where $\|\mathbf{z}\| = \|\mathbf{w}\| = 1$ and $\kappa \geq 0$, and similarly

$$C^*\mathbf{u} = \kappa \langle \mathbf{u}, \mathbf{z} \rangle \mathbf{w}, \quad \text{for all } \mathbf{u} \in \mathcal{H}_1.$$

The entries of the matrix C will be $C_{i,j} = \kappa \mathbf{z}_i \mathbf{w}_j$.

Remark 3.3.2. In [41], where $\mathcal{H}_1 = \mathcal{H}_2$, we take $C = \kappa P$, where $\kappa \in \mathbb{R}$, and P is a projection onto a one-dimensional subspace $Z = \text{Span}\{\mathbf{z}\}$, $\mathbf{z} \in \mathbb{R}^n$, $\|\mathbf{z}\| = 1$. Then, in the basis $\{\varphi_j\}$, P will have the matrix representation $(\langle \mathbf{z}, \varphi_i \rangle \langle \mathbf{z}, \varphi_j \rangle)_{i,j=1}^n$.

Let $\Phi_{X,\lambda}$ denote the eigenspace of a self-adjoint operator X corresponding to an eigenvalue λ , simple or multiple. Further denote, for any $\mathbf{f} \in \mathbb{R}^n$ with $\|\mathbf{f}\| = 1$,

$$\Gamma_{X,\mathbf{f}} := \{\lambda \in \text{Spec}(X) \mid \exists \phi \in \Phi_{X,\lambda} : \phi \neq 0 \text{ and } \langle \mathbf{f}, \phi \rangle = 0\},$$

$$\tilde{\Gamma}_{X,\mathbf{f}} := \{\lambda \in \text{Spec}(X) \mid \langle \mathbf{f}, \phi \rangle = 0 \quad \forall \phi \in \Phi_{X,\lambda}\}.$$

Here, X stands for either A or D , and \mathbf{f} stands for either \mathbf{z} or \mathbf{w} . For simplicity, denote

$$\begin{aligned} \Gamma_A &= \Gamma_{A,\mathbf{z}}, & \tilde{\Gamma}_A &= \tilde{\Gamma}_{A,\mathbf{z}}, \\ \Gamma_D &= \Gamma_{D,\mathbf{w}}, & \tilde{\Gamma}_D &= \tilde{\Gamma}_{D,\mathbf{w}}. \end{aligned}$$

Note that $\tilde{\Gamma}_{X,\mathbf{f}} \subseteq \Gamma_{X,\mathbf{f}}$. If λ is a simple eigenvalue of X , then $\dim(\Phi_{X,\lambda}) = 1$, and therefore $\lambda \in \Gamma_{X,\mathbf{f}} \iff \lambda \in \tilde{\Gamma}_{X,\mathbf{f}}$. Also, $\Gamma_{X,\mathbf{f}}$ contains all the multiple eigenvalues of X . This is due to the fact that in any linear subspace of dimension greater than one, one can find a non-trivial linear combination which is orthogonal to a given vector.

The orthogonal projection $P_{\mathbf{f}}$ of \mathcal{H} onto $\mathcal{S} = \text{Span}\{\mathbf{f}\}$ is a linear operator such that $P_{\mathbf{f}}\mathbf{y} \in \mathcal{S}$ for all $\mathbf{y} \in \mathcal{H}$, given by

$$P_{\mathbf{f}}\mathbf{y} = \langle \mathbf{y}, \mathbf{f} \rangle \mathbf{f}.$$

Let $Q_{\mathbf{f}} := I - P_{\mathbf{f}}$ be the orthogonal projection onto \mathcal{S}^\perp . For a self-adjoint operator $X : \mathcal{H} \rightarrow \mathcal{H}$, denote

$$\begin{aligned} X_{\parallel,\parallel} &= P_{\mathbf{f}}X|_{\mathcal{S}} : \mathcal{S} \rightarrow \mathcal{S}, & X_{\perp,\parallel} &= P_{\mathbf{f}}X|_{\mathcal{S}^\perp} : \mathcal{S}^\perp \rightarrow \mathcal{S}, \\ X_{\parallel,\perp} &= Q_{\mathbf{f}}X|_{\mathcal{S}} : \mathcal{S} \rightarrow \mathcal{S}^\perp, & X_{\perp,\perp} &= Q_{\mathbf{f}}X|_{\mathcal{S}^\perp} : \mathcal{S}^\perp \rightarrow \mathcal{S}^\perp. \end{aligned}$$

$P_{\mathbf{z}}$ and $P_{\mathbf{w}}$ will represent the orthogonal projection of \mathcal{H}_1 and \mathcal{H}_2 , onto $Z = \text{Span}\{\mathbf{z}\}$ and $W = \text{Span}\{\mathbf{w}\}$, respectively. The eigenvalues of $A_{\perp,\perp}$ and $D_{\perp,\perp}$ will be denoted by

$$\hat{\alpha}_1 \leq \dots \leq \hat{\alpha}_{n-1}, \quad \hat{\beta}_1 \leq \dots \leq \hat{\beta}_{m-1},$$

respectively, and their corresponding eigenvectors will be denoted by $\hat{\varphi}_k$ and $\hat{\psi}_l$, respectively.

Lemma 3.3.3. *The eigenvalues of X and $X_{\perp,\perp}$ always interlace, i.e. let $\lambda \in \text{Spec}(X)$ and $\hat{\lambda} \in \text{Spec}(X_{\perp,\perp})$, then for any $j \in \{1, \dots, \dim(X) - 1\}$,*

$$\lambda_j \leq \hat{\lambda}_j \leq \lambda_{j+1}.$$

3.3.2 Statement of the simple Chess Board Theorem

Assume for the moment that $\Gamma_A = \Gamma_D = \emptyset$, which in particular implies that all the eigenvalues of A and D are simple. Denote

$$x_0 := -\infty, \quad x_{2n} := \infty, \quad x_{2i-1} := \alpha_i, \quad x_{2k} := \hat{\alpha}_k,$$

and similarly for β ,

$$y_0 := -\infty, \quad y_{2m} := \infty, \quad y_{2j-1} := \beta_j, \quad y_{2l} := \hat{\beta}_l.$$

Then, the numbers x_0, \dots, x_{2n} divide the α -line into $2n$ intervals, finite or infinite, and similarly the numbers y_0, \dots, y_{2m} divide the β -line into $2m$ intervals. Combination of these lines divides the (α, β) -plane into rectangles, some of them semi-infinite,

$$\mathcal{R}_{p,q} := r_p \times r_q, \quad r_p := (x_{p-1}, x_p), \quad r_q := (y_{q-1}, y_q),$$

where $p = 1, \dots, 2n$ and $q = 1, \dots, 2m$, see Figure 3.4.

Theorem 3.3.4 (The Simple Chess Board Theorem). *Let $\Gamma_A = \Gamma_D = \emptyset$. Then all the real pair-eigenvalues (α, β) of \mathbb{M} lie on a family of curves $(\alpha, \beta(\alpha))$ with the following properties:*

- (a) *each curve may pass only through rectangles $\mathcal{R}_{p,q}$ with $p + q$ even;*
- (b) *each curve may cross from rectangle to rectangle only through the corner points (x_p, y_q) with $p + q$ odd;*

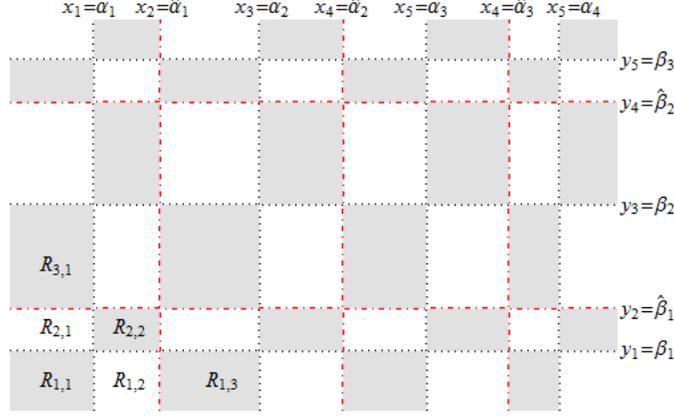


Figure 3.4: In the (α, β) -plane, black dotted and red dot-dashed lines in the vertical direction represent $\alpha = \alpha_i$ and $\alpha = \hat{\alpha}_k$, respectively; in the horizontal direction they represent $\beta = \beta_j$ and $\beta = \hat{\beta}_l$, respectively. Here $n = 4$ and $m = 3$, and the rectangles $\mathcal{R}_{p,q}$ with $p + q$ even are shaded.

(c) each curve $\beta(\alpha)$ is continuous in α except at eigenvalues of A ; at each eigenvalue of A exactly one curve blows up in the following sense: $\beta(\alpha) \rightarrow \pm\infty$ as $\alpha \rightarrow \alpha_i \pm 0$, $\alpha_i \in \text{Spec}(A)$;

(d) each curve $\beta(\alpha)$ is monotone decreasing in α on its domain of continuity; more precisely, we have

$$\frac{d\beta}{d\alpha} = -\kappa^2 \frac{\langle (A - \alpha)^{-2} \mathbf{z}, \mathbf{z} \rangle \langle (D - \beta)^{-1} \mathbf{w}, \mathbf{w} \rangle^2}{\langle (D - \beta)^{-2} \mathbf{w}, \mathbf{w} \rangle} < 0. \quad (3.18)$$

Remark 3.3.5. As α and β are in fact interchangeable, Theorem 3.3.4 can be equivalently reformulated in terms of curves $(\alpha(\beta), \beta)$ with the only modification being that exactly one curve $\alpha(\beta)$ blows up at each eigenvalue of B in the sense that $\alpha(\beta) \rightarrow \pm\infty$ as $\beta \rightarrow \beta_j \pm 0$, $\beta_j \in \text{Spec}(A)$.

3.3.3 Statement of the full Chess Board Theorem

In this section, we assume that either $\Gamma_A \neq \emptyset$ or $\Gamma_D \neq \emptyset$. Denote additionally, for $X : \mathcal{H} \rightarrow \mathcal{H}$,

$$\Delta_X := \{\lambda \in \text{Spec}(X) \mid \lambda \in \text{Spec}(X) \cap \text{Spec}(X_{\perp, \perp}) \quad \text{and} \quad \dim(\Phi_{X_{\perp, \perp}, \lambda}) > \dim(\Phi_{X, \lambda})\}.$$

We will state formally an analogue of Theorem 3.3.4 below, but we start with summarising the principle changes: first, we exclude from the dividing mesh the points of $\tilde{\Gamma}_A \setminus \Delta_A$ and $\tilde{\Gamma}_D \setminus \Delta_D$; and secondly, the real pair-spectrum of M will, in addition to the curves, contain the lines $(\Gamma_A \times \mathbb{R})$ and $(\mathbb{R} \times \Gamma_D)$.

More precisely, let $x_i, i = 1, \dots, s$, denote the points of

$$\left((\text{Spec}(A) \cup \text{Spec}(A_{\perp, \perp})) \setminus \tilde{\Gamma}_A \right) \cup \Delta_A$$

enumerated in increasing order without account of multiplicities, and similarly $y_j, j = 1, \dots, t$, denote the points of the analogue for D enumerated in increasing order without account of multiplicities. Set additionally $x_0 = y_0 = -\infty, x_{s+1} = y_{t+1} = +\infty$, and

$$\mathcal{R}_{p,q} = (x_{p-1}, x_p) \times (y_{q-1}, y_q), \quad p = 1, \dots, s+1, \quad q = 1, \dots, t+1.$$

Theorem 3.3.6 (The Full Chess Board Theorem). *All the real pair-eigenvalues (α, β) of \mathbb{M} lie either on the straight lines $(\Gamma_A \times \mathbb{R}) \cup (\mathbb{R} \times \Gamma_D)$ or on a family of curves $(\alpha, \beta(\alpha))$ with the following properties:*

- (a) *each curve may pass only through rectangles $\mathcal{R}_{p,q}$ with $p+q$ even;*
- (b) *each curve may cross from rectangle to rectangle only through the corner points (x_p, y_q) with $p+q$ odd;*
- (c) *each curve $\beta(\alpha)$ is continuous in α except at eigenvalues of A not belonging to $\tilde{\Gamma}_A$; at each such eigenvalue of A exactly one curve blows up in the following sense: $\beta(\alpha) \rightarrow \pm\infty$ as $\alpha \rightarrow \alpha_i \pm 0, \alpha_i \in \text{Spec}(A)$;*
- (d) *each curve $\beta(\alpha)$ is monotone decreasing in α on its domain of continuity with (3.18).*

Remark 3.3.7. The equation (3.16) is real analytic, therefore the solutions of (3.16) are also real analytic locally except at the points where the curves cross. We will see in Lemma 3.5.4 that when $\alpha \in \text{Spec}(A) \setminus \Gamma_A$ there are $m-1$ corresponding (α, β) pair-eigenvalues of \mathbb{M} which we can locate. In addition, as mentioned in Theorem 3.3.6(c), one curve blows up. Since each curve $\beta(\alpha)$ is monotone decreasing in α , it can be said that each curve lies its individual sequence of black rectangles, plus the one which blows up. Therefore these curves do not intersect as there is only one curve in each rectangle $\mathcal{R}_{p,q}$ with $p+q$ even. Thus, for every $\alpha \in \mathbb{C} \setminus \text{Spec}(A)$, there are m complex values $\beta(\alpha)$, and the corresponding curves can be chosen continuously in α since each curve is locally analytic in α . However, we note that we do not take into account of additional vertical (or horizontal) straight lines which are not in the mesh.

3.3.4 Limit cases

Only in this subsection, we will be denoting \mathbf{M} by \mathbf{M}_κ to indicate its dependence on κ . We state that when $\kappa \rightarrow 0$, the components of the real pair-eigenvalues of \mathbf{M}_κ approach the eigenvalues of A and D , and when $\kappa \rightarrow \infty$, they approach the eigenvalues of $A_{\perp,\perp}$ and $D_{\perp,\perp}$. The proof of the next result will be given in Section 3.5.

Theorem 3.3.8. *As $\kappa \rightarrow 0$, the real pair-eigenvalue spectrum of \mathbf{M}_κ converges to*

$$\mathcal{E}_{A,D} := (\text{Spec}(A) \times \mathbb{R}) \cup (\mathbb{R} \times \text{Spec}(D))$$

in the sense that $\forall \epsilon > 0 \exists \kappa_0 > 0$ such that $\forall (\alpha, \beta) \in \text{Spec}_p(\mathbf{M}_\kappa) \cap \mathbb{R}^2$ we have

$$\text{dist}((\alpha, \beta), \mathcal{E}_{A,D}) < \epsilon$$

whenever $\kappa < \kappa_0$.

As $\kappa \rightarrow \infty$, the real pair-eigenvalue spectrum of \mathbf{M}_κ converges to

$$\tilde{\mathcal{E}}_{A,D} := (\text{Spec}(A_{\perp,\perp}) \times \mathbb{R}) \cup (\mathbb{R} \times \text{Spec}(D_{\perp,\perp}))$$

in the sense that $\forall \epsilon > 0 \exists \kappa_0 > 0$ such that $\forall (\alpha, \beta) \in \text{Spec}_p(\mathbf{M}_\kappa) \cap \mathbb{R}^2$ we have

$$\text{dist}((\alpha, \beta), \tilde{\mathcal{E}}_{A,D}) < \epsilon$$

whenever $\kappa > \kappa_0$.

3.4 Auxiliary results

The statements in this section are for a single matrix X , and mostly very elementary. We shall use them later in the proof of the Chess Board Theorem. Let

$$\lambda_j \in \text{Spec}(X), \quad \phi_j \in \Phi_{X,\lambda_j}, \quad j = 1, \dots, \dim(X),$$

and

$$\hat{\lambda}_k \in \text{Spec}(X_{\perp,\perp}), \quad \hat{\phi}_k \in \Phi_{X_{\perp,\perp},\lambda_k}, \quad k = 1, \dots, \dim(X) - 1.$$

We shall frequently use the Fourier representation of the resolvent, for any $\mathbf{f} \in \mathbb{R}^n$ with $\|\mathbf{f}\| = 1$,

$$(X - \lambda)^{-1}\mathbf{f} = \sum_j \frac{\langle \mathbf{f}, \phi_j \rangle}{\lambda_j - \lambda} \phi_j, \quad \lambda \notin \text{Spec}(X). \quad (3.19)$$

We also set

$$R_X(\lambda, \mathbf{f}) := \langle (X - \lambda)^{-1}\mathbf{f}, \mathbf{f} \rangle = \sum_j \frac{|\langle \mathbf{f}, \phi_j \rangle|^2}{\lambda_j - \lambda}. \quad (3.20)$$

Lemma 3.4.1. *Let $\lambda \notin \text{Spec}(X)$ and $\mathbf{f} \neq 0$. Then*

$$R_X(\lambda, \mathbf{f}) = 0 \quad \Leftrightarrow \quad \lambda \in \text{Spec}(X_{\perp, \perp}) \quad \text{and} \quad (X - \lambda)^{-1} \mathbf{f} = c \widehat{\phi},$$

where $\widehat{\phi}$ is an eigenfunction of $X_{\perp, \perp}$ corresponding to λ and $c \neq 0$.

Proof. Set $\zeta = (X - \lambda)^{-1} \mathbf{f}$. Then

$$(X - \lambda)\zeta = \mathbf{f} \Leftrightarrow \begin{pmatrix} X_{\perp, \perp} - \lambda & X_{\parallel, \perp} \\ X_{\perp, \parallel} & X_{\parallel, \parallel} - \lambda \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{f} \end{pmatrix}, \quad (3.21)$$

where $\mathbf{q} = Q_f \zeta$ and $\mathbf{p} = P_f \zeta$. Note that $R_X(\lambda, \mathbf{f}) = \langle \zeta, \mathbf{f} \rangle = 0$ iff $\mathbf{p} = P_f \zeta = 0$. Substituting this into (3.21) gives us

$$\begin{cases} (X_{\perp, \perp} - \lambda)\mathbf{q} = \mathbf{0}, \\ X_{\perp, \parallel} \mathbf{q} = \mathbf{f}. \end{cases} \quad (3.22)$$

By the second equation, \mathbf{q} is non-zero, and then by the first equation $\lambda \in \text{Spec}(X_{\perp, \perp})$ and $\mathbf{q} = c \widehat{\phi}$, with $c \neq 0$. Also, we have

$$\mathbf{q} = Q_f \zeta = (I - P_f)\zeta = \zeta,$$

and so

$$\zeta = (X - \lambda)^{-1} \mathbf{f} = c \widehat{\phi}.$$

□

Lemma 3.4.2. $\lambda \in \Gamma_X$ if and only if $\lambda \in \text{Spec}(X) \cap \text{Spec}(X_{\perp, \perp})$.

Proof. If there exists an $\lambda \in \Gamma_X$, then there is an eigenfunction $\phi \in \Phi_{X, \lambda}$ such that $\langle \mathbf{f}, \phi \rangle = 0$, and therefore $P_f \phi = 0$ and so $Q_f \phi = \phi$. Thus

$$X_{\perp, \perp} \phi = Q_f X \phi = \lambda Q_f \phi = \lambda \phi,$$

and so $\lambda \in \text{Spec}(X) \cap \text{Spec}(X_{\perp, \perp})$.

On the other hand, let $\lambda \in \text{Spec}(X) \cap \text{Spec}(X_{\perp, \perp})$. Then

$$X \phi = \lambda \phi \quad \Rightarrow \quad \langle X \phi, \widehat{\phi} \rangle = \lambda \langle \phi, \widehat{\phi} \rangle = \lambda \langle Q_f \phi, \widehat{\phi} \rangle. \quad (3.23)$$

Also, since $\widehat{\phi} \perp \mathbf{f}$,

$$X \widehat{\phi} = X(\widehat{\phi} + 0\mathbf{f}) = X_{\perp, \perp} \widehat{\phi} + X_{\perp, \parallel} \widehat{\phi}, \quad (3.24)$$

therefore

$$\langle X \phi, \widehat{\phi} \rangle = \langle \phi, X \widehat{\phi} \rangle = \langle \phi, X_{\perp, \perp} \widehat{\phi} \rangle + \langle \phi, X_{\perp, \parallel} \widehat{\phi} \rangle$$

$$\begin{aligned}
&= \langle Q_{\mathbf{f}}\phi, X_{\perp,\perp}\widehat{\phi} \rangle + \langle P_{\mathbf{f}}\phi, X_{\perp,\parallel}\widehat{\phi} \rangle \\
&= \lambda \langle Q_{\mathbf{f}}\phi, \widehat{\phi} \rangle + \langle P_{\mathbf{f}}\phi, X_{\perp,\parallel}\widehat{\phi} \rangle
\end{aligned}$$

which implies by (3.23) that $\langle P_{\mathbf{f}}\phi, X_{\perp,\parallel}\widehat{\phi} \rangle = 0$. Now, if $P_{\mathbf{f}}\phi = 0$, then $\phi \perp \mathbf{f}$ so that $\lambda \in \Gamma_X$. If $X_{\perp,\parallel}\widehat{\phi} = 0$, then we have from (3.24) that $X\widehat{\phi} = \lambda\widehat{\phi}$, and therefore $\widehat{\phi}$ is an eigenfunction of X such that $\widehat{\phi} \perp \mathbf{f}$, so that $\lambda \in \Gamma_X$. \square

Lemma 3.4.3. *If $\lambda \in \text{Spec}(X) \setminus \widetilde{\Gamma}_X$, then $R_X(t, \mathbf{f})$ has a singularity at $t = \lambda$. The function $R_X(t, \mathbf{f})$ changes sign when t passes through an λ_j , or an $\widehat{\lambda}_k$.*

If $\lambda \in \widetilde{\Gamma}_X$, then $(X - \lambda)^{-1}\mathbf{f}$ exists, and $R_X(t, \mathbf{f})$ is continuous at $t = \lambda$. It changes sign at this λ if and only if additionally $\lambda \in \Delta_X$.

Proof. If $\lambda_j \in \text{Spec}(X) \setminus \widetilde{\Gamma}_X$, then there exists at least one $\phi_j \in \Phi_{X,\lambda}$ such that $\langle \mathbf{f}, \phi_j \rangle \neq 0$, and it can be seen from (3.20) that $R_X(t, \mathbf{f})$ goes to $\pm\infty$ as $\lambda \rightarrow \lambda_j \mp 0$. Furthermore, since $R_X(t, \mathbf{f})$ has zeros at $\lambda = \widehat{\lambda}_k$ by Lemma 3.4.1, and also is a continuous function except at the poles $\lambda = \lambda_j$, it changes sign every time z passes through $\widehat{\lambda}_j$ as well.

The second statement follows immediately from (3.20) and the fact that $\mathbf{f} \perp \Phi_{X,\lambda}$.

To show the last statement, we consider the following decomposition

$$\mathcal{H} = \Phi_{X,\lambda} \oplus Q_{\mathbf{f}}\Phi_{X,\lambda}^{\perp} \oplus P_{\mathbf{f}}\Phi_{X,\lambda}^{\perp},$$

where $\Phi_{X,\lambda}^{\perp}$ is the orthogonal complement of $\Phi_{X,\lambda}$ with respect to λ . Let $\dim(\Phi_{X,\lambda}) = d$ and therefore $\dim(Q_{\mathbf{f}}\Phi_{X,\lambda}^{\perp}) = \dim(X) - d - 1$ and $\dim(P_{\mathbf{f}}\Phi_{X,\lambda}^{\perp}) = 1$. Let $\widetilde{X} = X|_{\Phi_{X,\lambda}^{\perp}}$, then

$$X = \begin{pmatrix} \text{diag}(\lambda, \dots, \lambda) & 0 & 0 \\ 0 & \widetilde{X}_{\perp,\perp} & \widetilde{X}_{\parallel,\perp} \\ 0 & \widetilde{X}_{\perp,\parallel} & \widetilde{X}_{\parallel,\parallel} \end{pmatrix},$$

where the left corner block has dimension d . If $\lambda \in \Delta_X$ then $\lambda \in \text{Spec}(X) \cap \text{Spec}(X_{\perp,\perp})$ such that $\dim(\Phi_{X_{\perp,\perp},\lambda}) > \dim(\Phi_{X,\lambda}) = d$. Thus,

$$\lambda \in \Delta_X \Leftrightarrow \lambda \in \text{Spec}(\widetilde{X}_{\perp,\perp}) \quad \text{and} \quad \lambda \notin \text{Spec}(\widetilde{X}).$$

Therefore $R_{\widetilde{X}}(t, \mathbf{f})$ has zeros at $t = \lambda \in \Delta_X$ by Lemma 3.4.1, and the function $R_{\widetilde{X}}(t, \mathbf{f})$ changes sign at this λ . \square

Proof of Lemma 3.3.3. This lemma is known as Cauchy interlacing theorem. The proof is based on the variational principle. In finite dimensional case,

$$\langle X_{\perp,\perp}\mathbf{f}, \mathbf{f} \rangle = \langle Q_{\mathbf{f}}X\mathbf{f}, \mathbf{f} \rangle = \langle X\mathbf{f}, Q_{\mathbf{f}}\mathbf{f} \rangle = \langle X\mathbf{f}, \mathbf{f} \rangle,$$

since $Q_{\mathbf{f}} = Q_{\mathbf{f}}^*$ and $Q_{\mathbf{f}}\mathbf{f} = \mathbf{f}$, so the forms coincide, however the space is different. According to min-max theorem,

$$\lambda_j = \min_{U_1} \{ \max_{\mathbf{f}} \{ \langle X\mathbf{f}, \mathbf{f} \rangle \mid \mathbf{f} \in U_1 \setminus \{0\} \} \mid \dim(U_1) = j \},$$

$$\widehat{\lambda}_j = \min_{U_2} \{ \max_{\mathbf{f}} \{ \langle X_{\perp, \perp} \mathbf{f}, \mathbf{f} \rangle \mid \mathbf{f} \in U_2 \setminus \{0\} \} \mid \dim(U_2) = j \}.$$

We have the subspaces U_1 and U_2 of the same dimension, however U_1 contains a bigger collection of subspaces (it may additionally include elements from $P_{\mathbf{f}}\mathbf{f}$). Therefore, by taking \min over bigger set may be smaller, i.e.

$$\lambda_j \leq \widehat{\lambda}_j.$$

However, $\lambda_j = \widehat{\lambda}_j$ if and only if U_1 contains elements only from \mathbf{f}_{\perp} .

Looking at the other direction,

$$\lambda_{j+1} = \max_{U_1} \{ \min_{\mathbf{f}} \{ \langle X\mathbf{f}, \mathbf{f} \rangle \mid \mathbf{f} \in U_1 \setminus \{0\} \} \mid \dim(U_1) = n - j \},$$

$$\widehat{\lambda}_j = \max_{U_2} \{ \min_{\mathbf{f}} \{ \langle X_{\perp, \perp} \mathbf{f}, \mathbf{f} \rangle \mid \mathbf{f} \in U_2 \setminus \{0\} \} \mid \dim(U_2) = n - j \},$$

and for the same reason, by taking \max over bigger set may be bigger, i.e.

$$\widehat{\lambda}_j \leq \lambda_{j+1}.$$

□

3.5 Proofs of the main results

We proceed to the proof of Theorem 3.3.6; Theorem 3.3.4 follows from Theorem 3.3.6 immediately as a special case.

We first derive the characteristic equation of (3.13).

Theorem 3.5.1. *If $\alpha \notin \text{Spec}(A)$ and $\beta \notin \text{Spec}(D)$, then the characteristic equation of (3.13) for $\beta(\alpha)$ is*

$$\kappa^2 \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle \langle (D - \beta)^{-1} \mathbf{w}, \mathbf{w} \rangle = 1. \quad (3.25)$$

Proof. Re-writing the equation (3.16) as

$$(D - \beta)\mathbf{v} = C^*(A - \alpha)^{-1}C\mathbf{v}.$$

and then using the information that C is rank one, we obtain

$$(D - \beta)\mathbf{v} = C^*(A - \alpha)^{-1}C\mathbf{v},$$

$$\begin{aligned}
&= C^*(A - \alpha)^{-1} \kappa \langle \mathbf{v}, \mathbf{w} \rangle \mathbf{z} \\
&= \kappa^2 \langle \mathbf{v}, \mathbf{w} \rangle \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle \mathbf{w},
\end{aligned}$$

which implies

$$\mathbf{v} = \kappa^2 \langle \mathbf{v}, \mathbf{w} \rangle \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle (D - \beta)^{-1} \mathbf{w}.$$

Now since the term $\kappa^2 \langle \mathbf{v}, \mathbf{w} \rangle \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle$ is a constant, we can fix it as

$$\kappa^2 \langle \mathbf{v}, \mathbf{w} \rangle \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle = 1, \quad (3.26)$$

by setting

$$\mathbf{v} := (D - \beta)^{-1} \mathbf{w}. \quad (3.27)$$

Substituting (3.27) into (3.26), we arrive at (3.25). \square

Corollary 3.5.2. *Suppose $\alpha \notin \text{Spec}(A)$ and $\beta \notin \text{Spec}(D)$. Then the equation (3.25) is equivalent to the following one:*

$$\kappa^2 R_A(\alpha, \mathbf{z}) R_D(\beta, \mathbf{w}) = \kappa^2 \left(\sum_{i=1}^n \frac{|\langle \mathbf{z}, \boldsymbol{\varphi}_i \rangle|^2}{\alpha_i - \alpha} \right) \left(\sum_{j=1}^m \frac{|\langle \mathbf{w}, \boldsymbol{\psi}_j \rangle|^2}{\beta_j - \beta} \right) = 1. \quad (3.28)$$

Proof. The result yields by substituting $R_A(\alpha, \mathbf{z})$ and $R_D(\beta, \mathbf{w})$ into (3.25). \square

The next lemma shows that $(\Gamma_A \times \mathbb{C}) \cup (\mathbb{C} \times \Gamma_D) \subset \text{Spec}_p(\mathbf{M})$, strengthening in fact the claim of Theorem 3.3.6.

Lemma 3.5.3. *If $\alpha \in \Gamma_A$, then*

$$(\alpha, \beta) \in \text{Spec}_p(\mathbf{M}) \quad \text{for all } \beta \in \mathbb{C}.$$

Similarly, if $\beta \in \Gamma_D$, then

$$(\alpha, \beta) \in \text{Spec}_p(\mathbf{M}) \quad \text{for all } \alpha \in \mathbb{C}.$$

Proof. We prove the first of these statements, the second is similar. Let $\alpha \in \Gamma_A$, and let $\boldsymbol{\varphi} \in \Phi_{A, \alpha}$ such that $\langle \boldsymbol{\varphi}, \mathbf{z} \rangle = 0$. An immediate check shows that

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\varphi} \\ \mathbf{0} \end{pmatrix}$$

is a pair-eigenvector of \mathbf{M} for a pair-eigenvalue (α, β) with an arbitrary $\beta \in \mathbb{C}$. \square

In Lemma 3.5.3 we show what happens when $\alpha \in \Gamma_A$ or $\beta \in \Gamma_D$; our next result shows which points (α, β) may lie in $\text{Spec}_p(\mathbf{M})$ when α is an eigenvalue of A outside of Γ_A .

Lemma 3.5.4. *Let $\alpha \in \text{Spec}(A) \setminus \Gamma_A$, and $\beta \notin \Gamma_D$. Then $(\alpha, \beta) \in \text{Spec}_p(\mathbf{M})$ if and only if $\beta = \widehat{\beta} \in \text{Spec}(D_{\perp, \perp})$.*

Similarly, if $\beta \in \text{Spec}(D) \setminus \Gamma_D$, and $\alpha \notin \Gamma_A$, then $(\alpha, \beta) \in \text{Spec}_p(\mathbf{M})$ if and only if $\alpha = \widehat{\alpha} \in \text{Spec}(A_{\perp, \perp})$.

Proof. Once more, we only prove the first statement. Let $\alpha \in \text{Spec}(A) \setminus \Gamma_A$. Let us re-write (3.14), (3.15) as

$$(A - \alpha)\mathbf{u} = -\kappa\langle \mathbf{v}, \mathbf{w} \rangle \mathbf{z}, \quad (3.29)$$

$$(D - \beta)\mathbf{v} = -\kappa\langle \mathbf{u}, \mathbf{z} \rangle \mathbf{w}. \quad (3.30)$$

Multiplying (3.29) by $\varphi \in \Phi_{A, \alpha}$, we get

$$\langle (A - \alpha)\mathbf{u}, \varphi \rangle = \langle \mathbf{u}, (A - \alpha)\varphi \rangle = 0 = -\kappa\langle \mathbf{v}, \mathbf{w} \rangle \langle \mathbf{z}, \varphi \rangle.$$

Since $\alpha \notin \Gamma_A$, we have $\langle \mathbf{z}, \varphi \rangle \neq 0$, and so $\langle \mathbf{v}, \mathbf{w} \rangle = 0$ (and so $C\mathbf{v} = 0$), and by (3.29),

$$\mathbf{u} = a\varphi, \quad (3.31)$$

where the constant a may or may not be zero. Substituting now (3.31) into (3.30)

$$(D - \beta)\mathbf{v} = -\kappa a\langle \varphi, \mathbf{z} \rangle \mathbf{w}, \quad (3.32)$$

and since $\mathbf{v} \perp \mathbf{w}$, the equation (3.32) becomes

$$(D_{\perp, \perp} - \beta)\mathbf{v} + D_{\perp, \parallel}\mathbf{v} = -\kappa a\langle \varphi, \mathbf{z} \rangle \mathbf{w}. \quad (3.33)$$

Now, applying the projections $Q_{\mathbf{w}}$ and $P_{\mathbf{w}}$ to the result, we obtain

$$D_{\perp, \perp}\mathbf{v} = \beta\mathbf{v}, \quad (3.34)$$

$$D_{\perp, \parallel}\mathbf{v} = -\kappa a\langle \varphi, \mathbf{z} \rangle \mathbf{w}. \quad (3.35)$$

If $\beta \notin \text{Spec}(D_{\perp, \perp})$, then by (3.34), $\mathbf{v} = \mathbf{0}$, and thus $a = 0$, and so $\mathbf{u} = \mathbf{0}$, and $(\alpha, \beta) \notin \text{Spec}_p(\mathbf{M})$, proving the “only if” part of the statement.

If $\beta = \widehat{\beta} \in \text{Spec}(D_{\perp, \perp})$, and $\widehat{\psi} \in \Phi_{D_{\perp, \perp}, \widehat{\beta}}$, we choose $\mathbf{v} = b\widehat{\psi}$; we claim that we may choose constants a, b such that $a^2 + b^2 \neq 0$ to satisfy (3.35). After multiplying (3.35) by \mathbf{w} , it becomes

$$b\langle D_{\perp, \parallel}\widehat{\psi}, \mathbf{w} \rangle = -\kappa a\langle \varphi, \mathbf{z} \rangle. \quad (3.36)$$

The scalar product on the right-hand side is non-zero by our assumption $\alpha \notin \Gamma_A$. The scalar product on the left-hand side is non-zero since otherwise $D_{\perp, \parallel}\widehat{\psi}$, which acts on the space parallel to \mathbf{w} , is zero and by Lemma 3.5.3 $\widehat{\beta} \in \text{Spec } D$ with an eigenfunction $\widehat{\psi}$, and therefore $\beta \in \Gamma_D$ by Lemma 3.4.2, again contradicting our assumptions. Thus we can always choose a, b with $a^2 + b^2 \neq 0$ in order to satisfy (3.36). \square

We can now prove our main result.

Proof of the full Chess Board Theorem. The eigenvalues inside $(\Gamma_A \times \mathbb{R}) \cup (\mathbb{R} \times \Gamma_D)$ have been already accounted for by Lemma 3.5.3, so we will be working outside this set.

Recall the characteristic equation (3.28). Since it needs to be satisfied, $R_A(\alpha, \mathbf{z})$ and $R_D(\beta, \mathbf{w})$ have to have the same sign for real pair-eigenvalues. It can be seen from (3.20) that $R_A(\alpha, \mathbf{z})$ is positive when $\alpha < \alpha_1$, and by Lemma 3.4.3, it only changes sign every time when α passes through x_p , $p = 1, \dots, s$. Similarly, $R_D(\beta, \mathbf{w})$ is positive when $\beta < \beta_1$ and it only changes sign every time when β passes through y_q , $q = 1, \dots, t$. Thus the only allowed regions for real α and β are when $(\alpha, \beta) \in \mathcal{R}_{p,q}$ with $p + q$ even, proving, with account of Lemma 3.5.4, the statements (a) and (b).

Statement (c) follows immediately from (3.25) and Lemma 3.4.3.

To prove (d), we differentiate the characteristic equation (3.25) with respect to α , arriving at

$$\kappa^2 \langle (A - \alpha)^{-2} \mathbf{z}, \mathbf{z} \rangle \langle (D - \beta)^{-1} \mathbf{w}, \mathbf{w} \rangle + \kappa^2 \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle \langle (D - \beta)^{-2} \mathbf{w}, \mathbf{w} \rangle \frac{d\beta}{d\alpha} = 0,$$

so that

$$\frac{d\beta}{d\alpha} = - \frac{\langle (A - \alpha)^{-2} \mathbf{z}, \mathbf{z} \rangle \langle (D - \beta)^{-1} \mathbf{w}, \mathbf{w} \rangle}{\langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle \langle (D - \beta)^{-2} \mathbf{w}, \mathbf{w} \rangle},$$

and re-arranging with account of (3.25), we can re-write β' as in (3.18).

To see that $\beta' < 0$, we observe from (3.25) that $R_A(\alpha, \mathbf{z}) \neq 0$ and $R_D(\beta, \mathbf{w}) \neq 0$. Also,

$$\langle (A - \alpha)^{-2} \mathbf{z}, \mathbf{z} \rangle = \langle (A - \alpha)^{-1} \mathbf{z}, (A - \alpha)^{-1} \mathbf{z} \rangle = \|(A - \alpha)^{-1} \mathbf{z}\|,$$

which is always positive by (3.19), and similarly $\langle (D - \beta)^{-2} \mathbf{w}, \mathbf{w} \rangle > 0$, and therefore $d\beta/d\alpha < 0$. \square

Proof of Theorem 3.3.8. Let $\alpha \notin \text{Spec}(A)$ and $\beta \notin \text{Spec}(D)$. For a self-adjoint operator A , we have by Cauchy-Schwartz, if $\|\mathbf{z}\| = 1$,

$$|\langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle| \leq \|(A - \alpha)^{-1} \mathbf{z}\| \|\mathbf{z}\| \leq \|(A - \alpha)^{-1}\| = \frac{1}{\text{dist}(\alpha, \text{Spec}(A))}, \quad (3.37)$$

and similarly for D . By the characteristic equation (3.25), we have, as $\kappa \rightarrow 0$, that either

$$R_A(\alpha, \mathbf{z}) = \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle \rightarrow \infty$$

or

$$R_D(\beta, \mathbf{w}) = \langle (D - \beta)^{-1} \mathbf{w}, \mathbf{w} \rangle \rightarrow \infty,$$

which implies by (3.37) that either $\text{dist}(\alpha, \text{Spec}(A)) \rightarrow 0$ or $\text{dist}(\beta, \text{Spec}(D)) \rightarrow 0$. In other words, we have either α tends to an eigenvalue of A and β is arbitrary, or β tends to an eigenvalue of D and α is arbitrary. Then the first statement follows.

Similarly, if $\kappa \rightarrow \infty$, then again by (3.25) we have that either

$$R_A(\alpha, \mathbf{z}) = \langle (A - \alpha)^{-1} \mathbf{z}, \mathbf{z} \rangle \rightarrow 0$$

or

$$R_D(\beta, \mathbf{w}) = \langle (D - \beta)^{-1} \mathbf{w}, \mathbf{w} \rangle \rightarrow 0,$$

which implies by Lemma 3.4.1 that either $\alpha \rightarrow \hat{\alpha} \in \text{Spec}(A_{\perp, \perp})$ or $\beta \rightarrow \hat{\beta} \in \text{Spec}(D_{\perp, \perp})$. Then the second statement follows.

We note that our result holds under the hypothesis of the full Chess Board theorem since any point in Γ_A or Δ_A is always contained in $\text{Spec}(A) \cap \text{Spec}(A_{\perp, \perp})$, and similarly for D . \square

To finish the proof of the main theorem, it remains to show that the real pair-eigenvalues can only lie in rectangles $\mathcal{R}_{p,q}$ with $p + q$ even (except mesh lines). Actually we already mentioned in Remark 3.3.7 which rectangles are permitted and which are excluded. Nevertheless, we will show this case for the sake of completeness. As we know already by Lemma 3.5.4 that the eigenvalue curves can only cross through the mesh vertices, it is sufficient to indicate one rectangle with $p + q$ even which contains at least one real pair-eigenvalue. This will then determine which rectangles are permitted because of the crossings. In the next result, we show that for any $\kappa \neq 0$, one can always find a pair-eigenvalue in the region $\mathcal{R}_{2n, 2m}$ (or $\mathcal{R}_{s+1, t+1}$ when we have an eigenvalue with multiplicity greater than one).

Lemma 3.5.5. *Let α_n and β_m be the largest eigenvalue of A and D , respectively, which are in the mesh. For any $\alpha > \alpha_n$, $\exists \beta = \beta(\alpha) > \beta_m$ such that $(\alpha, \beta) \in \text{Spec}_p(\mathbf{M})$.*

Proof. Take $\alpha > \alpha_n$. Then the resolvent $(A - \alpha)^{-1}$ exists and is a negative operator. Moreover,

$$(\alpha, \beta) \in \text{Spec}_p(\mathbf{M}) \Leftrightarrow \beta \in \text{Spec}(T(\alpha)),$$

where $T(\alpha) = D - C^*(A - \alpha)^{-1}C$ is Hermitian. Thus, to prove the statement it remains to show that $T(\alpha)$ has an eigenvalue greater than β_m . Let \mathbf{v}_m be a normalised eigenvector of D corresponding to β_m . Then

$$\langle T(\alpha) \mathbf{v}_m, \mathbf{v}_m \rangle = \langle D \mathbf{v}_m, \mathbf{v}_m \rangle - \langle (A - \alpha)^{-1} \mathbf{w}_m, \mathbf{w}_m \rangle$$

where $\mathbf{w}_m = C\mathbf{v}_m$. If $\mathbf{w}_m \neq 0$, then by (3.20), we have

$$-\langle (A - \alpha)^{-1}\mathbf{w}_m, \mathbf{w}_m \rangle = \sum_{j=1}^n \frac{|\langle \mathbf{w}_m, \mathbf{u}_j \rangle|^2}{\alpha - \alpha_j} = \kappa^2 |\langle \mathbf{v}_m, \mathbf{w} \rangle|^2 \sum_{j=1}^n \frac{|\langle \mathbf{z}, \mathbf{u}_j \rangle|^2}{\alpha - \alpha_j},$$

which is always positive since $\alpha > \alpha_n$. Hence $\langle T(\alpha)\mathbf{v}_m, \mathbf{v}_m \rangle > \beta_m$. In that case, by variational principle $T(\alpha)$ has an eigenvalue $\beta(\alpha) > \beta_m$. Suppose $\mathbf{w}_m = 0$. Then

$$\mathbf{w}_m = C\mathbf{v}_m = \kappa \langle \mathbf{v}_m, \mathbf{w} \rangle \mathbf{z} = 0 \Leftrightarrow \mathbf{v}_m \perp \mathbf{w} \Leftrightarrow \beta_m \in \tilde{\Gamma}_D.$$

However, if $\beta_m \in \tilde{\Gamma}_D$ then β_m will not be in the mesh. Due to our construction, we do not take into account of the set $\tilde{\Gamma}$ in the mesh, and therefore $\mathbf{w}_m \neq 0$. \square

3.6 Examples

3.6.1 Example 1

As we mentioned earlier, the main motivation of this section comes from the particular non-self-adjoint problem which was considered in [19], with corresponding change of notations. Re-write the pencil problem as:

$$\begin{pmatrix} H_0^{(n)} - \alpha & \kappa C \\ \kappa C^* & H_0^{(m)} - \beta \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = 0, \quad (3.38)$$

where $(C)_{n,1} = 1$ and all other entries of C are zeros. We therefore set $\mathbf{z} = (0, \dots, 0, 1)^T$ and $\mathbf{w} = (1, 0, \dots, 0)^T$. When $\kappa = 1$, the problem (3.38) is equivalent to the pencil \mathcal{A}_c problem with (3.17), nevertheless we plot the spectrum for different values of κ .

The eigenvalues of $H_0^{(n)}$ are given by (2.37) and the eigenvalues of $(H_0^{(n)})_{\perp, \perp}$ are given by the same formula with n replaced by $n - 1$. We shall return to the investigation of the non-real pair-eigenvalues of this problem in Section 3.7.

Note that $\Gamma_{H_0^{(n)}} = \emptyset$ and the general spectral picture in the (α, β) -plane including the rectangular mesh can be seen in Figures 3.6 and Figure 3.11. We also illustrate in Figure 3.7 the real pair-eigenvalues by taking a wide range of κ values and superimposing them. We see that the results of the simple Chess Board Theorem hold. We also illustrate the limit cases in Figure 3.5 where we see that real pair-eigenvalues lie in the border of rectangular regions.

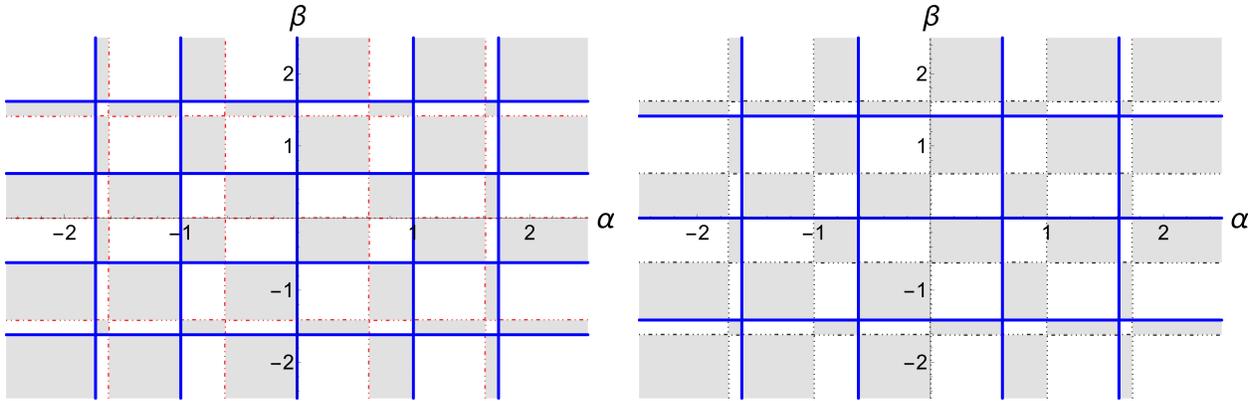


Figure 3.5: $\text{Spec}_p(\mathbf{M})$ when $A = H_0^{(5)}$ and $D = H_0^{(4)}$. Left: with $\kappa = 10^{-5}$. Right: with $\kappa = 10^5$.

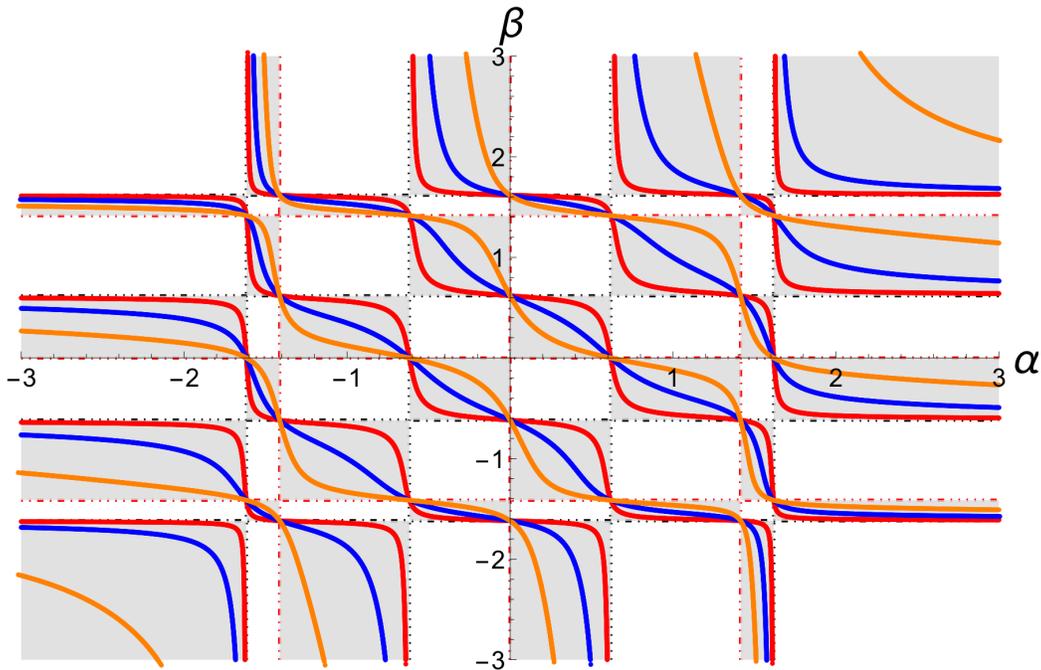


Figure 3.6: $\text{Spec}_p(\mathbf{M})$ when $A = D = H_0^{(4)}$ with $\kappa = 0.4$ (red curves), $\kappa = 1$ (blue curves) and $\kappa = 2$ (orange curves).

3.6.2 Example 2

This example illustrates the case when $\Gamma = \emptyset$. Let

$$A_2 = \text{diag}(-1, 2), \quad D_1 = \text{diag}(1, 3, 4). \quad (3.39)$$

Set

$$\mathbf{z} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \mathbf{w} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \quad (3.40)$$

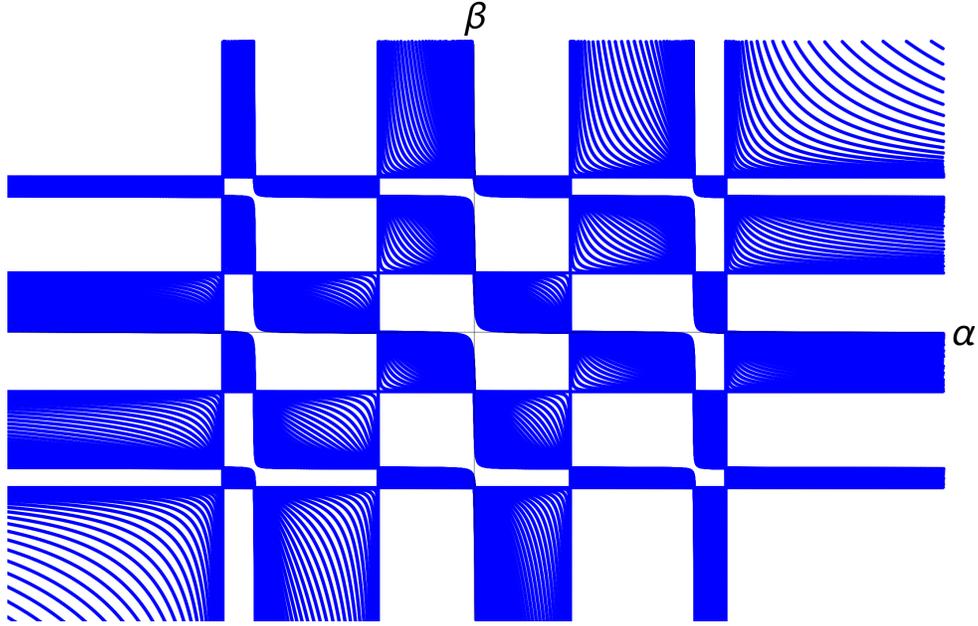


Figure 3.7: The superimposition of $\text{Spec}_p(\mathbf{M})$ when $A = D = H_0^{(4)}$ for the values of κ from 0.001 to 10 with the step-size of 0.1.

Then $\Gamma_{A_2} = \Gamma_{D_1} = \emptyset$. Also

$$\text{Spec}((A_2)_{\perp,\perp}) = \left\{ \frac{1}{2} \right\}, \quad \text{Spec}((D_1)_{\perp,\perp}) = \left\{ \frac{1}{3}(8 \pm \sqrt{7}) \right\}.$$

The spectral picture is illustrated in Figure 3.8(left), and we see that the simple Chess Board Theorem (Theorem 3.3.4) holds.

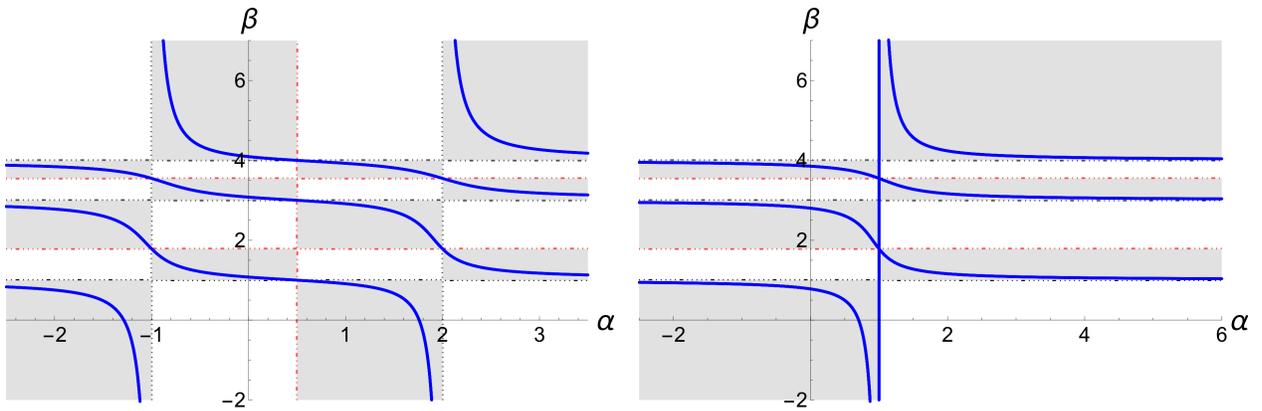


Figure 3.8: Left: $\text{Spec}_p(\mathbf{M})$ with $A = A_2$, $D = D_1$, and $\kappa = 1$. Right: $\text{Spec}_p(\mathbf{M})$ with $A = A_3$, $D = D_1$, and $\kappa = 3/4$.

Remark 3.6.1. In the rest of the examples, we set $D = D_1$ and w , as given in (3.39) and (3.40), thus $\Gamma_{D_1} = \emptyset$. We will consider different A and z in order to illustrate each special

case, therefore these changes will be seen in the vertical direction only.

3.6.3 Example 3

This example illustrates the case when $\Gamma \neq \emptyset$ and $\tilde{\Gamma} = \emptyset$. Consider

$$A_3 = \text{diag}(1, 1) \quad \text{and} \quad \mathbf{z} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (3.41)$$

Then $\Gamma_{A_3} = \{1\}$ and $\tilde{\Gamma}_{A_3} = \emptyset$. Also

$$\text{Spec}((A_3)_{\perp, \perp}) = \{1\}.$$

The spectral picture is illustrated in Figure 3.8(right). We see that $\text{Spec}_p(\mathbf{M})$ has an additional straight line at $\alpha = 1$, and there is also a blow-up at $\alpha = 1$. This line is included in the mesh since \mathbf{z} is orthogonal to one eigenvector but $\mathbf{z} \not\perp \Phi_{A_3, 1}$.

3.6.4 Example 4

This example illustrates the case when $\Gamma = \tilde{\Gamma} \neq \emptyset$. Consider

$$A_4 = \text{diag}(1, 4) \quad \text{and} \quad \mathbf{z} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Then $\Gamma_{A_4} = \tilde{\Gamma}_{A_4} = \{4\}$. Also

$$\text{Spec}((A_4)_{\perp, \perp}) = \{4\}.$$

The spectral picture is shown in Figure 3.9(left). It can be seen that there is an additional straight line passing through $\alpha = 4$ which is not included in the mesh since A_4 has simple eigenvalues and $\mathbf{z} \perp \Phi_{A_4, 4}$.

3.6.5 Example 5

This example illustrates the case when $\Gamma, \tilde{\Gamma} \neq \emptyset$ and $\Gamma \neq \tilde{\Gamma}$. Consider

$$A_5 = \text{diag}(-1, -1, 3, 3) \quad \text{and} \quad \mathbf{z} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Then $\Gamma_{A_5} = \{-1, 3\}$ and $\tilde{\Gamma}_{A_5} = \{-1\}$. Also

$$\text{Spec}((A_5)_{\perp, \perp}) = \{-1, 3\},$$

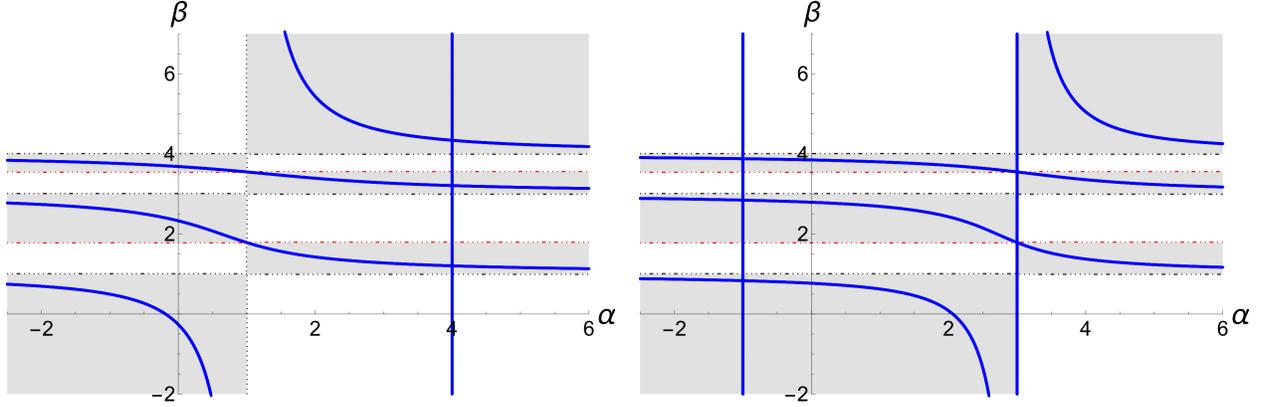


Figure 3.9: Left: $\text{Spec}_p(\mathbf{M})$ with $A = A_4$, $D = D_1$, and $\kappa = 3/2$. Right: $\text{Spec}_p(\mathbf{M})$ with $A = A_5$, $D = D_1$, and $\kappa = 4/3$.

where the eigenvalue -1 has multiplicity two. The spectral picture is shown in Figure 3.9(right). As expected, there are two additional vertical straight lines: at $\alpha = -1$, where there is no blow-up and the line is not included in the mesh since $\mathbf{z} \perp \Phi_{A_5, -1}$; and at $\alpha = 3$, where there is a blow-up and the line is included in the mesh since $\mathbf{z} \not\perp \Phi_{A_5, 3}$.

3.6.6 Example 6

Finally, this example illustrates the case when $\Delta \neq \emptyset$. Consider

$$A_6 = \text{diag}(1, 2, 2, 3) \quad \text{and} \quad \mathbf{z} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \quad (3.42)$$

Then $\Gamma_{A_6} = \tilde{\Gamma}_{A_6} = \{2\}$. Also

$$\text{Spec}((A_6)_{\perp, \perp}) = \{2\},$$

where the eigenvalue 2 has multiplicity three. The spectral picture is shown in Figure 3.10(right). Since $\mathbf{z} \perp \Phi_{A_6, 2}$, there is no blow-up at $\alpha = 2$. Nevertheless, this line is included in the mesh as $\Delta_{A_6} = \{2\}$, i.e. $\dim(\Phi_{(A_6)_{\perp, \perp}, 2}) > \dim(\Phi_{A_6, 2})$.

3.7 The non-real pair-eigenvalues of \mathbf{M}

We now turn our attention to the non-real pair eigenvalues of a two-parameter eigenvalue problem (3.13). Generally speaking, for every $\alpha \in \mathbb{C} \setminus \text{Spec}(A)$, we have either m corresponding $\beta \in \mathbb{C}$ which occurs under the restriction of the simple Chess Board Theorem,

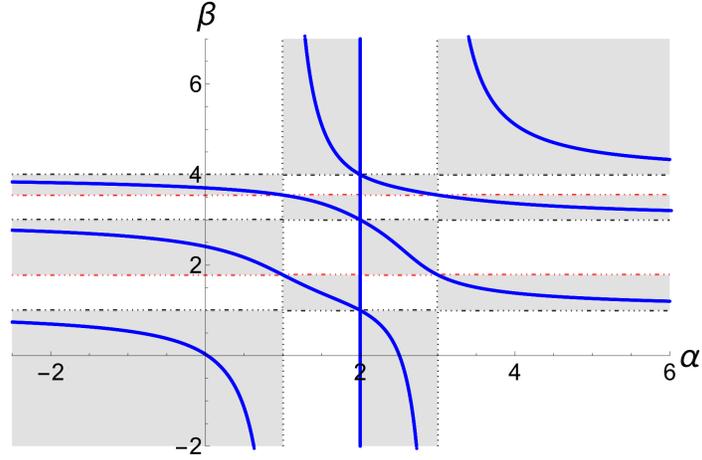


Figure 3.10: $\text{Spec}_p(\mathbf{M})$ with $A = A_6$, $D = D_1$, and $\kappa = 5/3$.

or infinitely many $\beta \in \mathbb{R}$ which occurs whenever Γ , $\tilde{\Gamma}$ or Δ is not equal to the empty set. We therefore limit our attention to the pair-eigenvalues subject to the additional restriction

$$\text{Im}(\alpha + \beta) = 0, \quad (3.43)$$

which is equivalent to introducing the additional restriction $c \in \mathbb{R}$ in the non-self-adjoint problem, see (3.17). For this reason, we introduce the following notation:

$$\widetilde{\text{Spec}}(\mathbf{M}) := \text{Spec}_p(\mathbf{M}) \cap \{(\alpha, \beta) \in \mathbb{C}^2 : \text{Im}(\alpha) + \text{Im}(\beta) = 0\}.$$

In addition, for brevity, we will work under the restrictions of the simple Chess Board Theorem.

Lemma 3.7.1. *The spectrum $\widetilde{\text{Spec}}(\mathbf{M})$ is invariant under the symmetry $(\alpha, \beta) \rightarrow (\bar{\alpha}, \bar{\beta})$.*

Proof. The result is true for any $\mathbf{M}(\alpha, \beta) = \mathbf{L} - \alpha\mathbf{V}_1 - \beta\mathbf{V}_2$ with self-adjoint coefficients \mathbf{L} , \mathbf{V}_1 and \mathbf{V}_2 : If (α, β) is a pair-eigenvalue of $\mathbf{M}(\alpha, \beta)$, then $\mathbf{L} - \alpha\mathbf{V}_1 - \beta\mathbf{V}_2$ is not invertible, therefore $(\mathbf{L} - \alpha\mathbf{V}_1 - \beta\mathbf{V}_2)^* = \mathbf{L} - \bar{\alpha}\mathbf{V}_1 - \bar{\beta}\mathbf{V}_2$ is not invertible and $(\bar{\alpha}, \bar{\beta})$ is a pair-eigenvalue of $\mathbf{M}(\alpha, \beta)$. \square

A general spectral picture of the non-self-adjoint problem considered in [19] is illustrated in the (α, β) -plane in Figure 3.11. Red curves depict the real parts of non-real pair-eigenvalues $\text{Re}\beta(\text{Re}\alpha)$ such that (3.43) holds, which keeps all $(\alpha, \beta) \in \mathbb{R}^2$ in the picture (shown in blue) and also some non-real pair-eigenvalues. In general, as can be seen from the examples which were considered in Section 3.6 there is no additional symmetry. Nevertheless, in our special example, we have the following result.

Corollary 3.7.2. Consider a two-parameter eigenvalue problem \mathbf{M} with $A = D = H_0^{(n)}$, $C = C^*$ with $(C)_{nn} = 1$ and all other entries of C are zeros. Then, in addition to the result of Lemma 3.7.1, the spectrum $\widetilde{\text{Spec}}(\mathbf{M})$ is invariant under the symmetry $(\alpha, \beta) \rightarrow (\beta, \alpha)$ and the symmetry $(\alpha, \beta) \rightarrow (-\beta, -\alpha)$.

Proof. We know by Lemma 3.1.3 that $\text{Spec}(\mathcal{A}_c)$ is invariant under the symmetries $\lambda \rightarrow -\lambda$ and $c \rightarrow -c$. We see by (3.17) that these symmetries correspond to $(\alpha, \beta) \rightarrow (\beta, \alpha)$ and $(\alpha, \beta) \rightarrow (-\beta, -\alpha)$, respectively. \square

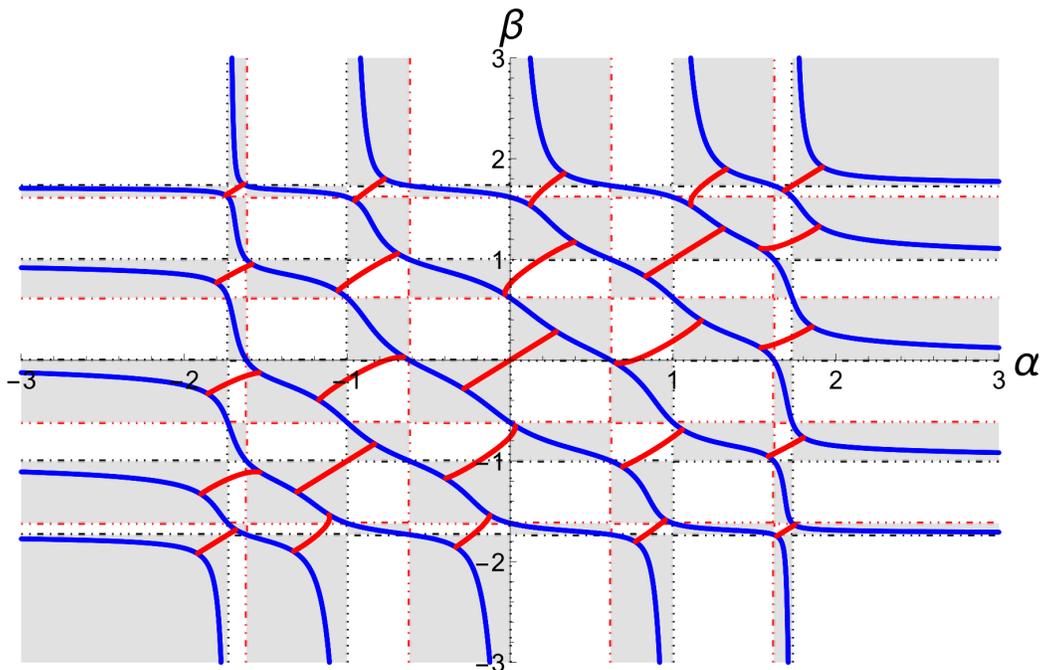


Figure 3.11: $\widetilde{\text{Spec}}(\mathbf{M})$ with $A = D = H_0$ and $C = B$ for $n = 5$.

The real and non-real eigenvalue curves $\lambda(c)$ may collide, with two possible types of collisions: those when two real eigenvalues collide and produce a complex conjugate pair, called Type-A, and those when a pair of complex conjugate eigenvalues collide and become real, called Type-B, see Figure 3.12 for equivalents in (α, β) -plane.

We gave an equivalent statement of Conjecture 1.3.3 in terms of a two-parameter eigenvalue problem in Theorem 1.3.4(i). We now turn to the proof of the result.

Proof of Theorem 1.3.4(i). Using the relation (3.17), we see that $\lambda \in \mathbb{C} \setminus \mathbb{R}$ if and only if $\alpha, \beta \in \mathbb{C} \setminus \mathbb{R}$. Consider the two-parameter eigenvalue problem $\mathbf{M}(\alpha, \beta)$ with $A = D = H_0^{(n)}$, $C = C^*$ with $(C)_{nn} = 1$ and all other entries of C are zeros. We know that any pencil problem of the form (1.10) and any two-parameter eigenvalue problem of the form (1.9)

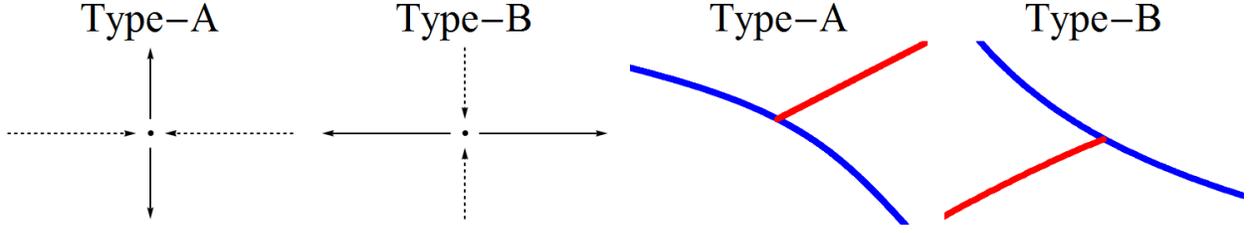


Figure 3.12: Left: the collisions in the $(\operatorname{Re}(\lambda), \operatorname{Im}(\lambda))$ -plane. Right: the collisions in the $(\operatorname{Re}(\alpha), \operatorname{Re}(\beta))$ -plane.

are equivalent by (1.14). Therefore this two-parameter problem $\mathbf{M}(\alpha, \beta)$ and (3.5) are likewise equivalent with $\alpha = \sigma$ and $\beta = -\tau$. If $c > 0$, then

$$|\alpha| = |\lambda - c| < 2, \quad |\beta| = |\lambda + c| < 2,$$

and if $c < 0$, then the inequalities will still hold by Corollary 3.7.2. \square

Unfortunately, we could not find much information about the non-real pair-eigenvalues which satisfy such bounds. Nevertheless, we found the collision locations in terms of derivative of $\beta(\alpha)$ with respect to α , and this holds not only for our pencil problem but also for any two-parameter eigenvalue problem with rank one C . Our first main result in this section is the following.

Lemma 3.7.3. *The collisions in $\widetilde{\operatorname{Spec}}(\mathbf{M})$ occur at the points where*

$$\frac{d\beta(\alpha)}{d\alpha} = -1.$$

Proof. Recall a two-parameter eigenvalue problem with the change of notation (3.17):

$$\begin{pmatrix} A - \lambda + c & C \\ C^* & D + \lambda + c \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0},$$

which can be written equivalently as

$$\mathbf{M}_\lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} A - \lambda & C \\ C^* & D + \lambda \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = -c \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}.$$

Considering $c(\lambda)$ and taking the derivative in each side of the spectral problem with respect to λ , we obtain

$$\begin{aligned} \mathbf{M}'_\lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} + \mathbf{M}_\lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}' &= -c' \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} - c \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}' \Leftrightarrow (\mathbf{M}_\lambda + c) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}' = (-c' - \mathbf{M}'_\lambda) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \\ &\Leftrightarrow (\mathbf{M}_\lambda + c) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}' = \left(-c' - \begin{pmatrix} -I & \\ & I \end{pmatrix} \right) \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \end{aligned}$$

which is solvable if and only if the left hand side of the last equation is orthogonal to $\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}$. Therefore multiplying by $\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}$ and bearing in mind $\|\mathbf{u}\| = \|\mathbf{v}\|$ by Corollary 3.1.8, we obtain

$$\begin{aligned} c' (\|\mathbf{u}\|^2 + \|\mathbf{v}\|^2) &= \left\langle \begin{pmatrix} I & \\ & -I \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}, \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} \right\rangle \\ &= \|\mathbf{u}\|^2 - \|\mathbf{v}\|^2 \\ &= 0. \end{aligned}$$

We show that the critical points occur when $\frac{dc}{d\lambda} = 0$; then using (3.17) gives

$$\frac{dc}{d\lambda} = \frac{\frac{dc}{d\alpha}}{\frac{d\lambda}{d\alpha}} = \frac{-\frac{1}{2} - \frac{1}{2}\beta'}{\frac{1}{2} - \frac{1}{2}\beta'} = 0 \quad \Leftrightarrow \quad \beta' = -1.$$

□

3.7.1 Limiting cases

If κ tends to zero, then the problem (3.13) becomes disjoint and the spectral picture can be understood easily. On the other hand, a very interesting phenomenon occurs when κ gets large; the spectral picture becomes more complicated. For instance, for some values of κ , non-real pair-eigenvalue collisions may occur, see Figure 3.13.

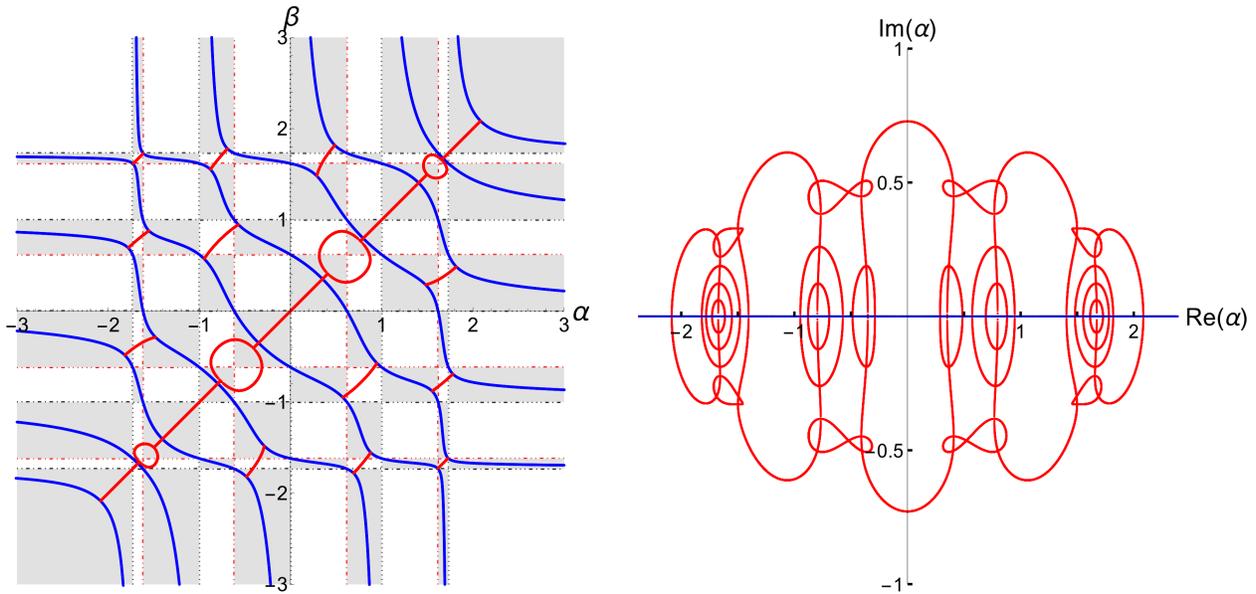


Figure 3.13: $\widetilde{\text{Spec}}(\mathbf{M})$ when $A = D = H_0$ with $n = 5$ for $\kappa = 1.37$. Left: in the $(\text{Re}(\alpha), \text{Re}(\beta))$ -plane. Right: in the $(\text{Re}(\alpha), \text{Im}(\alpha))$ -plane.

We know that if $\alpha \in \mathbb{R} \setminus (\text{Spec}(A) \cup \text{Spec}(A_{\perp, \perp}))$, then there are m corresponding real β 's such that

$$(\alpha, \beta_{\kappa}^{(1)}(\alpha)), \dots, (\alpha, \beta_{\kappa}^{(m)}(\alpha)) \in \widetilde{\text{Spec}}(\mathbf{M}).$$

Theorem 3.3.8 implies that as $\kappa \rightarrow \infty$, there are $(m - 1)$ corresponding β 's such that

$$\beta_{\kappa}^{(1)}(\alpha), \dots, \beta_{\kappa}^{(m-1)}(\alpha) \rightarrow \text{Spec}(D_{\perp, \perp}),$$

and m^{th} one goes to $\pm\infty$ where \pm depends on which block α lies in. For instance, as $\alpha \rightarrow \alpha_n + 0$, then $R_A(\alpha) \rightarrow -\infty$, and by (3.28) we obtain $R_D(\beta) \rightarrow -0$, and therefore $\beta(\alpha) \rightarrow +\infty$.

In addition to the real pair-eigenvalues, there are some non-real pair-eigenvalues and we cannot do the asymptotics for all of them. Nevertheless, if we restrict ourselves to $\widetilde{\text{Spec}}(\mathbf{M})$, there is one more family for which we will show the asymptotics as $\kappa \rightarrow \infty$. In the rest of this section, we shall analyse in more detail this family of pair-eigenvalues as κ tends to infinity.

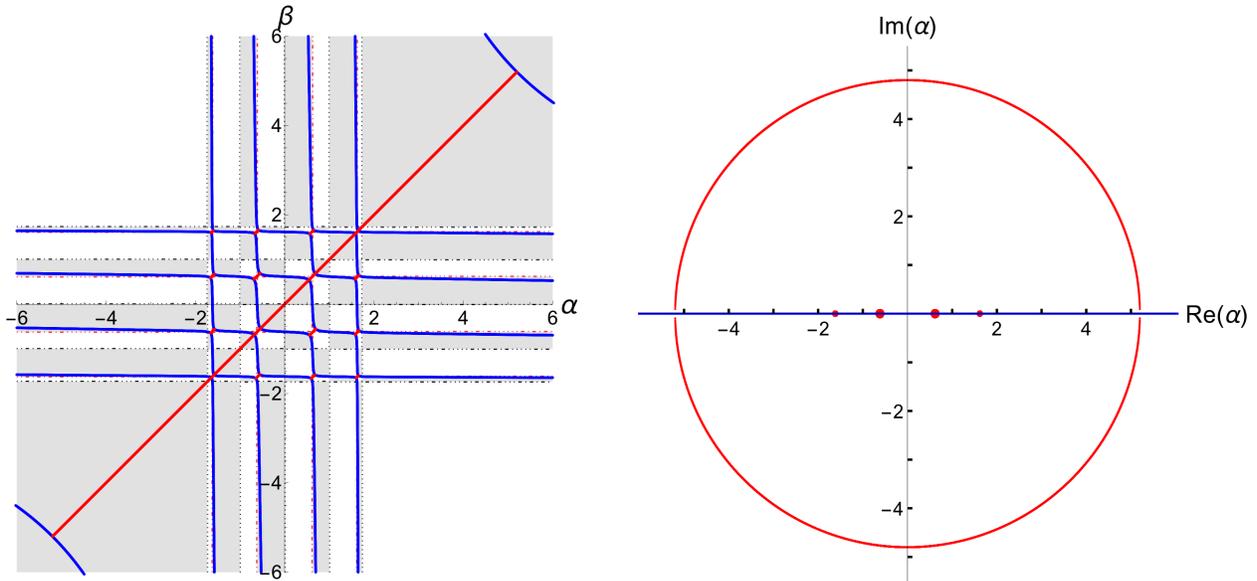


Figure 3.14: $\widetilde{\text{Spec}}(\mathbf{M})$ when $A = D = H_0$ with $n = 5$ for $\kappa = 5$. Left: in the $(\text{Re}(\alpha), \text{Re}(\beta))$ -plane. Right: in the $(\text{Re}(\alpha), \text{Im}(\alpha))$ -plane.

It can be seen in Figure 3.14 that for sufficiently large κ , α 's lie on a circle in the complex plane. Is it actually true that α 's and/or β 's lie on a circle? Can we figure out what the circle is? Is it always the case or only for this particular example? In the next theorem, which is one of the main results of this section, we will show that it is indeed the case; namely, if we take two circles of sufficiently large radius κ , centred at $A_{\parallel, \parallel}$ in the α -plane and $D_{\parallel, \parallel}$ in the β -plane, then each point in the first circle will be approximately the

first component of the large eigenvalue-pair, and each point in the second circle will be approximately the second component of the same eigenvalue-pair. Note that $A_{\parallel,\parallel}$, $D_{\parallel,\parallel} \in \mathbb{R}$ and can be computed as

$$A_{\parallel,\parallel} \mathbf{z} = \langle A \mathbf{z}, \mathbf{z} \rangle \mathbf{z}, \quad D_{\parallel,\parallel} \mathbf{w} = \langle D \mathbf{w}, \mathbf{w} \rangle \mathbf{w},$$

which are some constants proportional to \mathbf{z} and \mathbf{w} , respectively.

Theorem 3.7.4. *As $\nu = \frac{1}{\kappa} \rightarrow 0$, there exist a family of pair-eigenvalues $(\alpha, \beta) \in \widetilde{\text{Spec}}(\mathbf{M})$ such that*

$$|\alpha - A_{\parallel,\parallel}|^2 = \kappa^2 + O(\nu^2), \quad (3.44)$$

$$|\beta - D_{\parallel,\parallel}|^2 = \kappa^2 + O(\nu^2), \quad (3.45)$$

or more precisely, for any $t \in \mathbb{R}$, $(\alpha_t, \beta_t) \in \widetilde{\text{Spec}}(\mathbf{M})$, where

$$\alpha_t = e^{it} \nu^{-1} + a_1 + O(\nu), \quad \beta_t = e^{-it} \nu^{-1} + b_1 + O(\nu), \quad (3.46)$$

and a_1 and b_1 , which are in general depending on t , satisfy

$$\text{Re}((a_1 - A_{\parallel,\parallel})e^{-it}) = 0, \quad \text{Re}((b_1 - D_{\parallel,\parallel})e^{it}) = 0.$$

The next result will be useful in the proof of Theorem 3.7.4.

Lemma 3.7.5. *Let $c \in \mathbb{C} \setminus \{0\}$ arbitrary constant. Then the system*

$$\begin{pmatrix} c & 1 \\ 1 & 1/c \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} = \begin{pmatrix} s \\ t \end{pmatrix}$$

has a non-trivial solution if and only if

$$ct - s = 0.$$

Proof. Re-writing as a system of two equations

$$cp + q = s,$$

$$p + (1/c)q = t,$$

and leaving p alone in the second equation and substituting into the first equation gives

$$c(t - (1/c)q) + q = s \Leftrightarrow ct - s = 0.$$

□

Proof of Theorem 3.7.4. First, we prove the expansions given in (3.46). Then will deduce the formulas (3.44) and (3.45). Take

$$\alpha = \kappa a, \quad \beta = \kappa b, \quad \nu = \frac{1}{\kappa},$$

where $a, b \in \mathbb{C}$ and we let $\nu \rightarrow 0$. Then the equation (3.14) and (3.15) can be re-written as

$$\left. \begin{aligned} A\mathbf{u} + \kappa\langle\mathbf{v}, \mathbf{w}\rangle\mathbf{z} &= \alpha\mathbf{u} \\ D\mathbf{v} + \kappa\langle\mathbf{u}, \mathbf{z}\rangle\mathbf{w} &= \beta\mathbf{v} \end{aligned} \right\} \Leftrightarrow \left\{ \begin{aligned} \nu A\mathbf{u} + \langle\mathbf{v}, \mathbf{w}\rangle\mathbf{z} &= a\mathbf{u} \\ \nu D\mathbf{v} + \langle\mathbf{u}, \mathbf{z}\rangle\mathbf{w} &= b\mathbf{v} \end{aligned} \right.$$

and we are seeking a solution of the form

$$\begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \sum_{k=0}^{\infty} \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} \nu^k, \quad \begin{pmatrix} a \\ b \end{pmatrix} = \sum_{k=0}^{\infty} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \nu^k.$$

At order $O(\nu^0)$, we have

$$\left. \begin{aligned} \langle\mathbf{v}_0, \mathbf{w}\rangle\mathbf{z} &= a_0\mathbf{u}_0 \\ \langle\mathbf{u}_0, \mathbf{z}\rangle\mathbf{w} &= b_0\mathbf{v}_0 \end{aligned} \right\} \quad (3.47)$$

which implies that

$$\begin{aligned} \mathbf{u}_0 &= c_0\mathbf{z}, \\ \mathbf{v}_0 &= d_0\mathbf{w}, \end{aligned}$$

where c_0, d_0 are constants. Substituting these into (3.47) gives us

$$\left. \begin{aligned} d_0 &= a_0c_0 \\ c_0 &= b_0d_0 \end{aligned} \right\}$$

and therefore

$$a_0b_0 = 1. \quad (3.48)$$

Since we can always re-scale the eigenfunctions, we set $c_0 = 1$ and write the first terms as

$$\begin{pmatrix} \mathbf{u}_0 \\ \mathbf{v}_0 \end{pmatrix} = \begin{pmatrix} \mathbf{z} \\ a_0\mathbf{w} \end{pmatrix}.$$

Using the additional restriction $\text{Im}(a_0 + b_0) = 0$, we write

$$\begin{aligned} a_0 &= a_{0,r} + ia_{0,i} \\ b_0 &= b_{0,r} - ia_{0,i} \end{aligned}$$

and substituting these into (3.48) yields

$$\left. \begin{aligned} a_{0,r} &= b_{0,r} \\ a_{0,r}b_{0,r} + a_{0,i}^2 &= 1 \end{aligned} \right\}$$

which implies

$$a_0 = e^{it}, \quad b_0 = e^{-it} \quad (3.49)$$

for arbitrary $t \in \mathbb{R}$. At order $O(\nu^1)$, we have

$$\left. \begin{aligned} A\mathbf{u}_0 + \langle \mathbf{v}_1, \mathbf{w} \rangle \mathbf{z} &= a_0 \mathbf{u}_1 + a_1 \mathbf{u}_0 \\ D\mathbf{v}_0 + \langle \mathbf{u}_1, \mathbf{z} \rangle \mathbf{w} &= b_0 \mathbf{v}_1 + b_1 \mathbf{v}_0 \end{aligned} \right\} \Leftrightarrow \left\{ \begin{aligned} A\mathbf{z} + \langle \mathbf{v}_1, \mathbf{w} \rangle \mathbf{z} &= e^{it} \mathbf{u}_1 + a_1 \mathbf{z} \\ e^{it} D\mathbf{w} + \langle \mathbf{u}_1, \mathbf{z} \rangle \mathbf{w} &= e^{-it} \mathbf{v}_1 + e^{it} b_1 \mathbf{w} \end{aligned} \right. \quad (3.50)$$

Now separating vectors orthogonal and parallel to \mathbf{z} and \mathbf{w} in (3.50), we get

$$A_{\parallel, \perp} \mathbf{z} = e^{it} Q_{\mathbf{z}} \mathbf{u}_1 \quad (3.51)$$

$$(A_{\parallel, \parallel} - a_1) \mathbf{z} - e^{it} P_{\mathbf{z}} \mathbf{u}_1 + \langle \mathbf{v}_1, \mathbf{w} \rangle \mathbf{z} = 0 \quad (3.52)$$

$$e^{it} D_{\parallel, \perp} \mathbf{w} = e^{-it} Q_{\mathbf{w}} \mathbf{v}_1 \quad (3.53)$$

$$(e^{it} D_{\parallel, \parallel} - e^{it} b_1) \mathbf{w} - e^{-it} P_{\mathbf{w}} \mathbf{v}_1 + \langle \mathbf{u}_1, \mathbf{z} \rangle \mathbf{w} = 0 \quad (3.54)$$

Now, write (3.52) and (3.54) as a system

$$\begin{pmatrix} -e^{it} & 1 \\ 1 & -e^{-it} \end{pmatrix} \begin{pmatrix} \langle \mathbf{u}_1, \mathbf{z} \rangle \\ \langle \mathbf{v}_1, \mathbf{w} \rangle \end{pmatrix} = \begin{pmatrix} a_1 - A_{\parallel, \parallel} \\ e^{it}(b_1 - D_{\parallel, \parallel}) \end{pmatrix}. \quad (3.55)$$

By Lemma 3.7.5, the system (3.55) has a non-trivial solution if and only if

$$(a_1 - A_{\parallel, \parallel})e^{-it} + (b_1 - D_{\parallel, \parallel})e^{it} = 0.$$

Separating real and imaginary parts as $a_1 = a_{1,r} + ia_{1,i}$ and $b_1 = b_{1,r} - ia_{1,i}$, we obtain

$$\begin{aligned} &\Leftrightarrow (a_{1,r} - A_{\parallel, \parallel} + ia_{1,i})(\cos t - i \sin t) + (b_{1,r} - D_{\parallel, \parallel} - ia_{1,i})(\cos t + i \sin t) = 0 \\ &\Leftrightarrow \begin{cases} (a_{1,r} - A_{\parallel, \parallel} + b_{1,r} - D_{\parallel, \parallel}) \cos t + (a_{1,i} + a_{1,i}) \sin t = 0 \\ (a_{1,i} - a_{1,i}) \cos t + (-a_{1,r} + A_{\parallel, \parallel} + b_{1,r} - D_{\parallel, \parallel}) \sin t = 0 \end{cases} \\ &\Leftrightarrow \begin{cases} (a_{1,r} - A_{\parallel, \parallel} + b_{1,r} - D_{\parallel, \parallel}) \cos t + 2a_{1,i} \sin t = 0 \\ (a_{1,r} - A_{\parallel, \parallel} - b_{1,r} + D_{\parallel, \parallel}) \sin t = 0 \end{cases} \end{aligned} \quad (3.56)$$

From the second equation of (3.56), we obtain

$$a_{1,r} - A_{\parallel, \parallel} = b_{1,r} - D_{\parallel, \parallel}, \quad (3.57)$$

and substituting this into the first equation of (3.56) we obtain

$$2(a_{1,r} - A_{\parallel, \parallel}) \cos t + 2a_{1,i} \sin t = 0 \quad \Leftrightarrow \quad \operatorname{Re}[(a_1 - A_{\parallel, \parallel})e^{-it}] = 0, \quad (3.58)$$

and similarly

$$2(b_{1,r} - D_{\parallel,\parallel}) \cos t - 2a_{1,i} \sin t = 0 \quad \Leftrightarrow \quad \operatorname{Re}[(b_1 - D_{\parallel,\parallel})e^{it}] = 0. \quad (3.59)$$

Now, substituting a_0 and a_1 into α , we have

$$\begin{aligned} \alpha &= \nu^{-1}a = a_0\nu^{-1} + a_1 + O(\nu^1) \\ &= e^{it}\nu^{-1} + a_1 + O(\nu), \end{aligned}$$

and similarly, substituting b_0, b_1 into β , we have

$$\begin{aligned} \beta &= \nu^{-1}b = b_0\nu^{-1} + b_1 + O(\nu^1) \\ &= e^{-it}\nu^{-1} + b_1 + O(\nu), \end{aligned}$$

where a_1 and b_1 satisfies (3.58) and (3.59), respectively.

We now prove (3.44), the second statement (3.45) is similar. Using the expansion for α in (3.46) we get

$$\begin{aligned} |\alpha - A_{\parallel,\parallel}|^2 &= |\kappa a - A_{\parallel,\parallel}|^2 \\ &= |\nu^{-1}(a_0 + \nu a_1) - A_{\parallel,\parallel}|^2 + O(\nu^2) \\ &= |\nu^{-1}e^{it} + a_1 - A_{\parallel,\parallel}|^2 + O(\nu^2) \\ &= |\nu^{-1}|^2 |e^{it} + \nu(a_1 - A_{\parallel,\parallel})|^2 + O(\nu^2) \\ &= \nu^{-2} [1 + 2\nu \operatorname{Re}[(a_1 - A_{\parallel,\parallel})e^{-it}]] + O(\nu^2) \\ &= \nu^{-2} + O(\nu^2) \\ &= \kappa^2 + O\left(\frac{1}{\kappa^2}\right), \end{aligned}$$

where we used (3.58) and $|x + y|^2 = |x|^2 + |y|^2 + 2\operatorname{Re}(\bar{x}y)$. □

We see from Figure 3.14 that when $A = D$, the large non-real pair-eigenvalue seems to occur on the line $\operatorname{Re}(\alpha) \cong \operatorname{Re}(\beta)$ which is equivalent to $\operatorname{Re}(\lambda) = 0$ in the non-self-adjoint problem. We now formally state this result as a corollary.

Corollary 3.7.6. *Let $A = D$. Then there exists a pair eigenvalue $(\alpha, \beta) \in \widetilde{\operatorname{Spec}}(\mathbf{M})$ such that*

$$\operatorname{Re}(\alpha) = \operatorname{Re}(\beta) + O(\kappa^{-2}),$$

i.e.

$$\alpha = \bar{\beta} + O(\kappa^{-2}).$$

Proof. This follows immediately from (3.49) and (3.57). □

3.7.2 Examples

In this section, we apply the limit results to the examples given in Section 3.6. Most examples produce similar plots so we only mention three of them here. In each graph, we also plot a circle of radius κ , centred at $A_{\parallel,\parallel}$ in the α -plane and $D_{\parallel,\parallel}$ in the β -plane, and both indicated by a black circle.

First, consider $A = D = H_0$, and take $n = 7$. Then $(H_0)_{\parallel,\parallel} = 0$ and the behaviour of the non-real eigenvalues in the α -plane can be seen in Figure 3.15. Since we take $A = D$, we plot the figures only in the α -plane as figures in the β -plane are identical. The figure illustrates that one family of non-real pair-eigenvalues approaches a circle as κ increases, whereas the rest of the non-real eigenvalues get smaller and eventually become real.

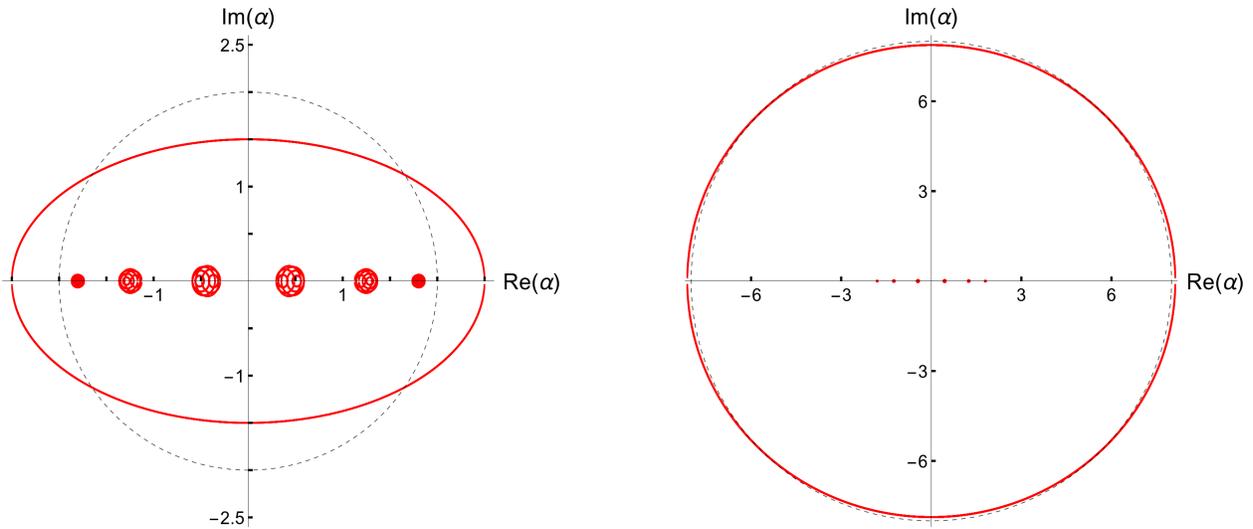


Figure 3.15: $\widetilde{\text{Spec}}(\mathbf{M}) \setminus \mathbb{R}^2$ (red curves) in the α -plane with $A = D = H_0$ for $n = 7$. Left: $\kappa = 2$ and $\mathcal{D}(0, 2)$ (black dashed circle). Right: $\kappa = 8$ and $\mathcal{D}(0, 8)$ (black dashed circle).

Now, we consider some two-parameter eigenvalue examples given in Section 3.6. As a second illustration, consider Example 3, i.e. take $A = A_3$ with $\mathbf{z} = (1, 0)^T$ as in (3.41), and $D = D_1$ with $\mathbf{w} = 1/\sqrt{3}(1, 1, 1)^T$ as in (3.39). Then

$$(A_3)_{\parallel,\parallel} = 1, \quad (D_1)_{\parallel,\parallel} = 8/3.$$

The limiting non-real eigenvalue behaviour for large κ can be seen as expected in Figure 3.16.

Third, we consider Example 6, i.e. take $A = A_6$ with $\mathbf{z} = 1/\sqrt{2}(1, 0, 0, 1)^T$ as in (3.42), and $D = D_1$ with $\mathbf{w} = 1/\sqrt{3}(1, 1, 1)^T$ as in (3.39). Then $(A_6)_{\parallel,\parallel} = 2$. The limiting non-real eigenvalue behaviour can be seen in Figure 3.17.

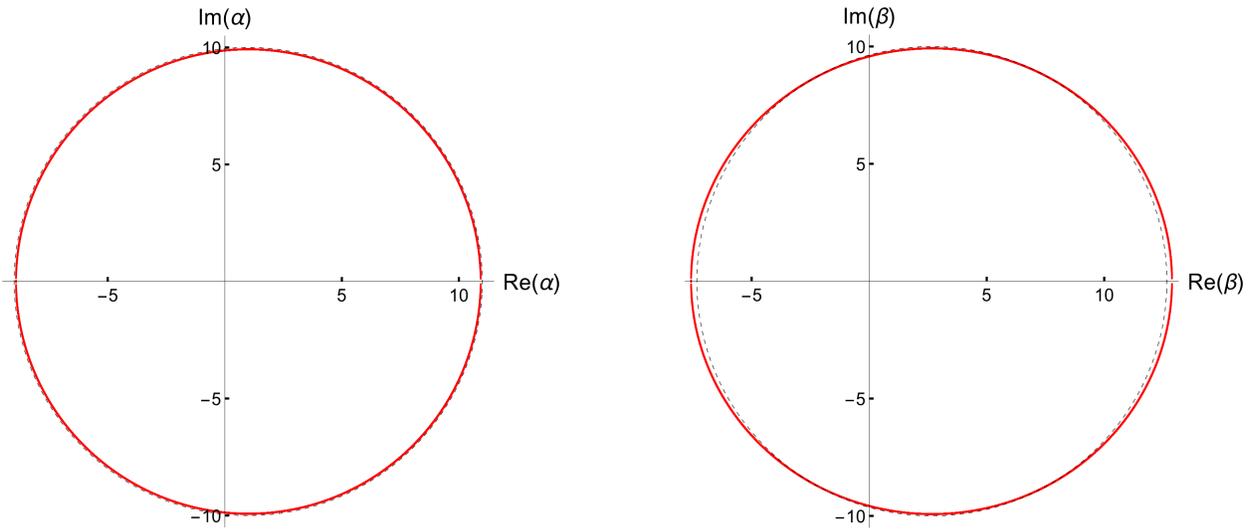


Figure 3.16: $\widetilde{\text{Spec}}(\mathbf{M}) \setminus \mathbb{R}^2$ (red curves) with $A = A_3$ and $D = D_1$ for $\kappa = 10$. Left: $\mathcal{D}(1, 10)$ (black dashed circle) in the α plane. Right: $\mathcal{D}(8/3, 10)$ (black dashed circle) in the β -plane.

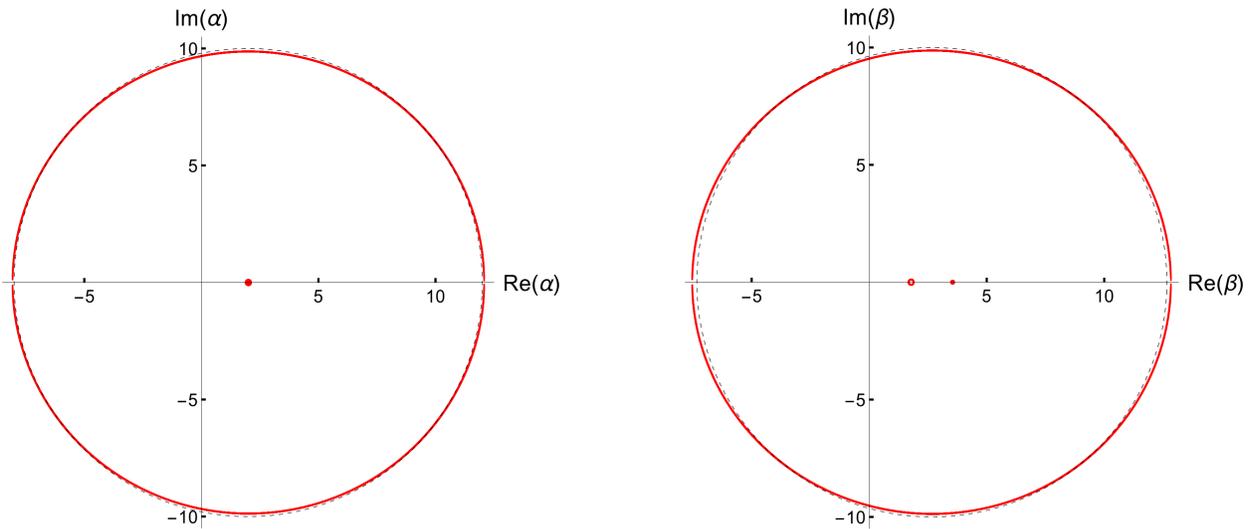


Figure 3.17: $\widetilde{\text{Spec}}(\mathbf{M}) \setminus \mathbb{R}^2$ (red curves) with $A = A_6$ and $D = D_1$ for $\kappa = 10$. Left: $\mathcal{D}(2, 10)$ (black dashed circle) in the α plane. Right: $\mathcal{D}(8/3, 10)$ (black dashed circle) in the β -plane.

Chapter 4

Bounds for the eigenvalues of \mathcal{A}_c

In this chapter, we turn our attention to the linear pencil problem (3.3) and try to answer some open questions about the non-real eigenvalues of \mathcal{A}_c . These questions were first raised by Davies and Levitin [19]. We will try to treat the problem (3.3) differently in order to gain meaningful information. We start by re-writing the characteristic equation of \mathcal{A}_c in numerous ways in Section 4.1. In addition, Conjecture 1.3.3 can be reformulated in various ways and we mention three of them in Section 4.2. Section 4.3 contains a full proof of the conjecture when $n = 2$ and $n = 3$. We will see below that the conjecture is non-trivial in these cases. Section 4.4 uses asymptotic methods to locate the non-real eigenvalues of \mathcal{A}_c when c goes to zero.

Finally, Section 4.5 applies the useful tools introduced in Chapter 2 to our pencil problem. We study finite ratios of Chebyshev polynomials of the second kind $U_n(\zeta)$ in Section 4.2.1. We shall see that known ratio asymptotic estimates mentioned in Section 4.5.2 are not sufficient when applied to the ratio $U_{n+1}(\zeta)/U_n(\zeta)$. Therefore we will look at the finite ratios of $U_n(\zeta)$ in more detail to obtain better estimates. The results we will obtain are still inadequate to answer the open questions, nonetheless we believe that these estimates are useful. We conclude the chapter in Section 4.5.3 with a detailed discussion of the well-known Gershgorin-type results when applied to our particular problem.

4.1 Different representation of the operator pencil \mathcal{A}_c

Our goal in this section is to treat the linear pencil problem (3.3) in various ways by writing several variations of the characteristic equation.

4.1.1 Explicit expressions for eigenfunctions of \mathcal{A}_c

The problem (3.5) can be re-written as

$$(H_0 - \sigma I)\mathbf{u} = -B\mathbf{v}, \quad (4.1)$$

$$(H_0 + \tau I)\mathbf{v} = -B\mathbf{u}. \quad (4.2)$$

Recall the relation $F_j(\zeta) = U_j(\zeta/2)$, where U_j is the Chebyshev polynomial of the second kind, and that the function F_j satisfies the recurrence relation (2.35).

Lemma 4.1.1. *Let $\zeta \notin \text{Spec}(H_0)$, and let \mathbf{w} solve*

$$(H_0^{(n)} - \zeta I)\mathbf{w} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}. \quad (4.3)$$

Then

$$\mathbf{w} = \mathbf{w}(\zeta) = -\frac{1}{F_n(\zeta)} \begin{pmatrix} F_0(\zeta) \\ F_1(\zeta) \\ \vdots \\ F_{n-2}(\zeta) \\ F_{n-1}(\zeta) \end{pmatrix} = -\frac{F_{n-1}(\zeta)}{F_n(\zeta)} \begin{pmatrix} F_0(\zeta)/F_{n-1}(\zeta) \\ F_1(\zeta)/F_{n-1}(\zeta) \\ \vdots \\ F_{n-2}(\zeta)/F_{n-1}(\zeta) \\ 1 \end{pmatrix}$$

with

$$\|\mathbf{w}(\zeta)\|^2 = \frac{\mathcal{F}_n(\zeta)}{|F_n(\zeta)|^2},$$

where

$$\mathcal{F}_n(\zeta) := \sum_{j=0}^{n-1} |F_j(\zeta)|^2. \quad (4.4)$$

Proof. The equation (4.3) is written in components as

$$\begin{aligned} w_2 - \zeta w_1 &= 0 \\ w_{j-1} - \zeta w_j + w_{j+1} &= 0, \quad \text{for } j = 2, \dots, (n-1), \\ w_{n-1} - \zeta w_n &= 1. \end{aligned}$$

Substituting $w_j = -\frac{F_{j-1}(\zeta)}{F_n(\zeta)}$ we see that all n equations hold by (2.35). □

Corollary 4.1.2. Let $\mathbf{u}, \mathbf{v}, \sigma, \tau$ solve (4.1)-(4.2), and let $\sigma, \tau \notin \{\mu_n, \dots, \mu_1\}$. Then

$$\mathbf{u} = -v_n \mathbf{w}(\sigma) = \frac{v_n}{F_n(\sigma)} \begin{pmatrix} F_0(\sigma) \\ F_1(\sigma) \\ \vdots \\ F_{n-1}(\sigma) \end{pmatrix},$$

$$\mathbf{v} = -u_n \mathbf{w}(-\tau) = \frac{u_n}{F_n(\tau)} \begin{pmatrix} (-1)^n F_0(\tau) \\ (-1)^{n+1} F_1(\tau) \\ \vdots \\ -F_{n-1}(\tau) \end{pmatrix}.$$

Proof. Immediate from (4.1)-(4.2) and Lemma 4.1.1. □

Lemma 4.1.3. Let $\mathbf{u}, \mathbf{v}, \sigma, \tau$ solve (4.1)-(4.2), and in addition let $\sigma, \tau \notin \{\mu_n, \dots, \mu_1\}$ and $\|\mathbf{u}\| = 1$. Then $\lambda = (\sigma + \tau)/2$ is a simple eigenvalue of \mathcal{A}_c , and

$$F_{n-1}(\sigma)F_{n-1}(\tau) + F_n(\sigma)F_n(\tau) = 0, \quad (4.5)$$

where

$$\sigma = \lambda - c, \quad \tau = \lambda + c.$$

Moreover

$$|v_n|^2 = \frac{|F_n(\sigma)|^2}{\mathcal{F}_n(\sigma)} = \frac{|F_{n-1}(\tau)|^2}{\mathcal{F}_n(\tau)}, \quad (4.6)$$

$$|u_n|^2 = \frac{|F_n(\tau)|^2}{\mathcal{F}_n(\tau)} = \frac{|F_{n-1}(\sigma)|^2}{\mathcal{F}_n(\sigma)}. \quad (4.7)$$

Additionally,

$$\mathbf{u} = \frac{e^{is}}{\sqrt{\mathcal{F}_n(\sigma)}} \begin{pmatrix} F_0(\sigma) \\ F_1(\sigma) \\ \vdots \\ F_{n-1}(\sigma) \end{pmatrix}, \quad \mathbf{v} = \frac{e^{it}}{\sqrt{\mathcal{F}_n(\tau)}} \begin{pmatrix} (-1)^n F_0(\tau) \\ (-1)^{n+1} F_1(\tau) \\ \vdots \\ -F_{n-1}(\tau) \end{pmatrix}.$$

for some $s, t \in \mathbb{R}$.

Proof. By Corollary 4.1.2,

$$u_n = v_n \frac{F_{n-1}(\sigma)}{F_n(\sigma)}, \quad v_n = -u_n \frac{F_{n-1}(\tau)}{F_n(\tau)},$$

which implies (4.5). The eigenvalue is geometrically simple since the eigenspace is one-dimensional (with u_n or v_n being a simple parameter). By Lemma 2.1.3, we know that

$\|\mathbf{u}\| = \|\mathbf{v}\|$. The first equalities in each of (4.6) and (4.7) are then obtained from the normalising conditions

$$\begin{aligned}\|\mathbf{v}\|^2 &= |u_n|^2 \|\mathbf{w}(-\tau)\|^2 = |u_n|^2 \frac{\mathcal{F}_n(\tau)}{|F_n(\tau)|^2} = 1, \\ \|\mathbf{u}\|^2 &= |v_n|^2 \|\mathbf{w}(\sigma)\|^2 = |v_n|^2 \frac{\mathcal{F}_n(\sigma)}{|F_n(\sigma)|^2} = 1.\end{aligned}$$

The second ones are obtained from writing normalising conditions as

$$\|\mathbf{v}\|^2 = |v_n|^2 \sum_{j=1}^n \frac{|v_j|^2}{|v_n|^2} = |v_n|^2 \frac{\mathcal{F}_n(\tau)}{|F_{n-1}(\tau)|^2} = 1,$$

and similarly for \mathbf{u} . [Remark: the second inequalities in (4.6) and (4.7) can be also deduced from the first ones and (4.5).] The expressions for \mathbf{u} and \mathbf{v} result from a substitution. \square

Remark 4.1.4. It would be nice to obtain additional restrictions on σ and τ from the fact that the quantities in (4.6) and (4.7) should be less than one. Unfortunately this is not the case - the numerics of the contour plot of the RH sides in (4.6) and (4.7) show that the curves on which $\frac{|F_n(\tau)|^2}{\mathcal{F}_n(\tau)} = 1$ protrude (by a small amount) into the domain $|\tau| > 2$ (or $\text{Re}(\tau) > 2$) for $n \geq 4$. These curves are illustrated in Figure 4.1 as n increases. Note that this is because the construction above does not use the crucial condition $\text{Im}(\sigma) = \text{Im}(\tau)$.

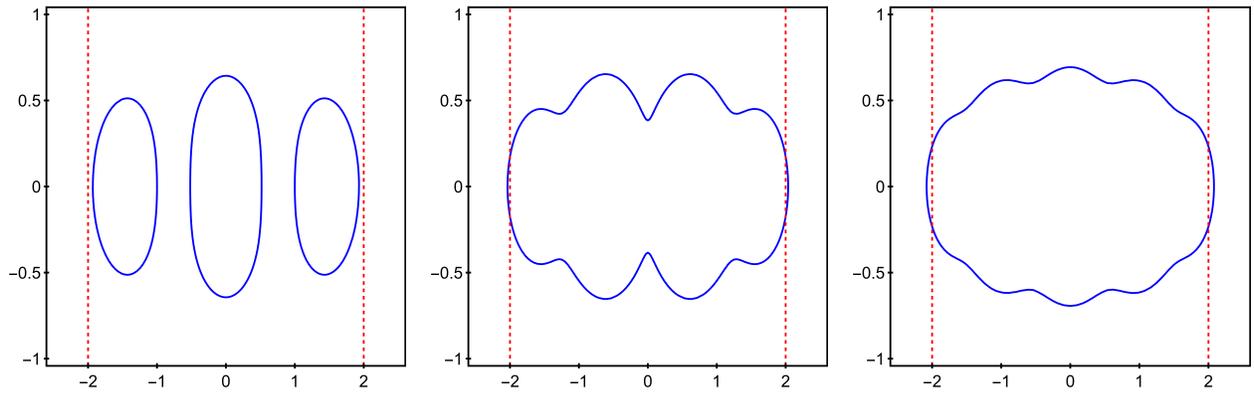


Figure 4.1: Contour plots of $\frac{|F_n(\tau)|^2}{\mathcal{F}_n(\tau)} = 1$ (blue curves) in the $(\text{Re}(\tau), \text{Im}(\tau))$ -plane and $\text{Re}(\tau) = \pm 2$ (red dashed lines) for $n = 3$, $n = 4$ and $n = 5$ from left to right.

4.1.2 Mapping $z + 1/z$

Let $\lambda \in \text{Spec}(\mathcal{A}_c)$. We use the following substitution

$$\lambda - c = \sigma := z + \frac{1}{z}, \quad \lambda + c = \tau := w + \frac{1}{w}, \quad (4.8)$$

where z and w are some complex numbers. Note that each λ corresponds to two values of z (which are inverses of each other) and two values of w (which are also inverses of each other). These values are the solutions of the quadratic equations

$$z^2 - (\lambda - c)z + 1 = 0, \quad (4.9)$$

$$w^2 - (\lambda + c)w + 1 = 0, \quad (4.10)$$

respectively. If λ is non-real, then we define z and w to be the unique solutions of (4.9) and (4.10), respectively, which satisfy

$$|z| > 1, \quad |w| > 1. \quad (4.11)$$

Define the meromorphic function $f_n : \mathbb{C}^2 \rightarrow \mathbb{C}$ by

$$f_n(z, w) = (z^{n+1} - z^{-n-1})(w^{n+1} - w^{-n-1}) + (z^n - z^{-n})(w^n - w^{-n}). \quad (4.12)$$

The next result is the characteristic polynomial of the pencil \mathcal{A}_c , deduced in [19], as an explicit complex polynomial equation in two variables.

Lemma 4.1.5 ([19, Lemma 2.4]). *Let z, w, λ be related by (4.9)-(4.10). If $\sigma = z + z^{-1} \neq \pm 2$ and $\tau = w + w^{-1} \neq \pm 2$, then*

$$\det(H_c^{(2n)} - \lambda S) = (-1)^n \frac{f_n(z, w)}{(z - z^{-1})(w - w^{-1})}.$$

Remark 4.1.6. Lemma 4.1.5 is not the exact statement of Lemma 2.4 in [19]. To be precise, Davies and Levitin [19] constructed the characteristic polynomial of a linear pencil $H_0^{(N)} - \lambda S_{m,n;\sigma,\tau}$ where $S_{m,n;\sigma,\tau}$ is the diagonal matrix

$$S_{m,n;\sigma,\tau} = \begin{pmatrix} \sigma I_m & \\ & \tau I_n \end{pmatrix},$$

and what we state here is the special case when $m = n$ and $-\tau$ instead of τ .

Let $\mathcal{D}(o, r)$ be the disk of radius r around a point o , that is,

$$\mathcal{D}(o, r) := \{\zeta \in \mathbb{C} : |\zeta - o| < r\},$$

and let $\partial\mathcal{D}(o, r)$ be the boundary of the disk $\mathcal{D}(o, r)$. In addition, define the families of meromorphic function $G_n : \mathbb{C} \rightarrow \mathbb{C}$ by

$$G_n(\xi) := \frac{\xi^{n+1} - \xi^{-n-1}}{\xi^n - \xi^{-n}}. \quad (4.13)$$

Now, we quote another result from [19] which relates the eigenvalues of the pencil \mathcal{A} to the function f_n and G_n .

Theorem 4.1.7 ([19, Theorem 2.3]). *Let $\lambda \in \mathbb{C} \setminus \{-2 - c, -2 + c, 2 - c, 2 + c\}$ and let λ, z, w be related by (4.8)-(4.11). Then*

(a) λ is an eigenvalue of the pencil \mathcal{A}_c if and only if

$$f_n(z, w) = 0. \quad (4.14)$$

(b) If λ is an eigenvalue of \mathcal{A}_c , then it is real if and only if both z and w lie in the set

$$\partial\mathcal{D}(0, 1) \cup (\mathbb{R} \setminus \{0\}).$$

(c) If $\lambda \notin \mathbb{R}$ then λ is an eigenvalue of \mathcal{A}_c if and only if

$$G_n(z)G_n(w) = -1. \quad (4.15)$$

Remark 4.1.8. Looking at the imaginary parts of (4.8), we see that

$$\operatorname{Im}\lambda = \operatorname{Im}\left(z + \frac{1}{z}\right) = \operatorname{Im}\left(w + \frac{1}{w}\right),$$

and re-arranging this we obtain

$$\operatorname{Im}\lambda = \operatorname{Im}(z) \left(1 - \frac{1}{|z|^2}\right) = \operatorname{Im}(w) \left(1 - \frac{1}{|w|^2}\right). \quad (4.16)$$

If $\lambda \in \mathbb{C} \setminus \mathbb{R}$, then using $|z| > 1$ and $|w| > 1$ implies that corresponding $\operatorname{Im}(z)$ and $\operatorname{Im}(w)$ are of the same sign.

Remark 4.1.9. Let $\lambda \in \mathbb{R}$. Then Theorem 4.1.7(b) immediately follows from (4.16). In addition, we have from (4.9) and (4.10) that

$$z = \frac{\lambda - c \pm \sqrt{(\lambda - c)^2 - 4}}{2}, \quad w = \frac{\lambda + c \pm \sqrt{(\lambda + c)^2 - 4}}{2}. \quad (4.17)$$

It follows from Lemma 3.1.1 that $|\lambda| \geq 2 + |c|$ is impossible. Also it can be seen from (4.17) with account of Theorem 4.1.7(b) that

$$\lambda \in (-2 - c, -2 + c] \Leftrightarrow z \in \mathbb{R}, \quad w \in \partial\mathcal{D}(0, 1), \quad (4.18)$$

$$\lambda \in (-2 + c, 2 - c) \Leftrightarrow z \in \partial\mathcal{D}(0, 1), \quad w \in \partial\mathcal{D}(0, 1), \quad (4.19)$$

$$\lambda \in [2 - c, 2 + c) \Leftrightarrow z \in \partial\mathcal{D}(0, 1), \quad w \in \mathbb{R}. \quad (4.20)$$

In addition, Theorem 4.1.7(b) states that if $\lambda \in \mathbb{R}$, and z and/or w are non-real, then they lie on the unit circle $\partial\mathcal{D}(0, 1)$.

4.1.3 \mathcal{A}_c in the basis of eigenfunctions of H_0

Let the matrix Ψ have the entries $(\psi_{j,k})_{j,k=1}^n = \left(\sqrt{2/(n+1)} \sin(\pi jk/(n+1)) \right)_{j,k=1}^n$, i.e.

$$\Psi := \sqrt{\frac{2}{n+1}} \begin{pmatrix} \sin\left(\frac{\pi}{n+1}\right) & \sin\left(\frac{2\pi}{n+1}\right) & \cdots & \sin\left(\frac{\pi n}{n+1}\right) \\ \sin\left(\frac{2\pi}{n+1}\right) & \sin\left(\frac{4\pi}{n+1}\right) & & \vdots \\ \vdots & & \ddots & \\ \sin\left(\frac{\pi n}{n+1}\right) & \cdots & & \sin\left(\frac{\pi n^2}{n+1}\right) \end{pmatrix}. \quad (4.21)$$

Since the columns of Ψ are normalised eigenfunctions of H_0 which is Hermitian, Ψ is a unitary matrix, i.e.

$$\Psi = \Psi^* = \Psi^T = \Psi^{-1}.$$

In the orthonormal basis

$$\left\{ \begin{pmatrix} \psi_1 \\ \mathbf{0} \end{pmatrix}, \dots, \begin{pmatrix} \psi_n \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \mathbf{0} \\ \psi_1 \end{pmatrix}, \dots, \begin{pmatrix} \mathbf{0} \\ \psi_n \end{pmatrix} \right\},$$

where $\mathbf{0}$ represents the zero vector in \mathbb{R}^n , the problem (3.5) can be re-written as follows.

Lemma 4.1.10. *Using the change of basis matrix $\text{diag}(\Psi, \Psi)$, the spectral problem (3.5) is equivalent to the problem*

$$\begin{pmatrix} \mu_1 - \sigma & & & \psi_{1,n}\psi_{n,n} & \cdots & \psi_{1,n}\psi_{1,n} \\ & \ddots & & \vdots & & \vdots \\ & & \mu_n - \sigma & \psi_{n,n}\psi_{n,n} & \cdots & \psi_{n,n}\psi_{1,n} \\ \psi_{1,n}\psi_{n,n} & \cdots & \psi_{1,n}\psi_{1,n} & \mu_1 + \tau & & \\ \vdots & & \vdots & & \ddots & \\ \psi_{n,n}\psi_{n,n} & \cdots & \psi_{n,n}\psi_{1,n} & & & \mu_n + \tau \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \\ v_n \\ \vdots \\ v_1 \end{pmatrix} = \mathbf{0}. \quad (4.22)$$

Proof. Note that $(\text{diag}(\Psi, \Psi))^{-1} = \text{diag}(\Psi, \Psi)$. Consider the problem (3.5). Since for any non-singular matrix X , the spectrum of A and $X^{-1}AX$ are the same, the matrix on the left-hand side of (3.5) can be written in the following alternative form:

$$\begin{pmatrix} \Psi & \\ & \Psi \end{pmatrix} \begin{pmatrix} H_0 - \sigma I & B \\ B & H_0 + \tau I \end{pmatrix} \begin{pmatrix} \Psi \\ \Psi \end{pmatrix} = \begin{pmatrix} \Psi H_0 \Psi - \sigma I & \Psi B \Psi \\ \Psi B \Psi & \Psi H_0 \Psi + \tau I \end{pmatrix}. \quad (4.23)$$

Calculating

$$\tilde{H}_0 := \Psi H_0 \Psi = \text{diag}(\mu_1, \dots, \mu_n), \quad (4.24)$$

$$\tilde{B} := \Psi B \Psi = (\psi_{n,j}\psi_{k,n})_{j,k=1}^n \quad (4.25)$$

Substituting these into (4.23) and recalling that $\psi_{j,k} = \psi_{k,j}$, we arrive at (4.22). \square

We will apply Gershgorin Theorem to the problem (4.22) and deduce the corresponding Gershgorin set in Section 4.5.3.3.

4.2 Reformulating Conjecture 1.3.3 in different forms

As can be seen in Theorem 1.3.4, there are several ways to reformulate Conjecture 1.3.3. Our aim in this section is to re-write the conjecture by using the different forms of characteristic equation.

4.2.1 Ratios of orthogonal polynomials

Define the family of meromorphic function $\tilde{F}_n : \mathbb{C} \rightarrow \mathbb{C}$ by

$$\tilde{F}_n(\zeta) := \frac{F_n(\zeta)}{F_{n-1}(\zeta)}. \quad (4.26)$$

In fact, the function $\tilde{F}_n(\zeta)$ is equal to the ratios of Chebyshev polynomials of the second kind $U_n(\zeta/2) = F_n(\zeta)$. Then the following recurrence relation is immediate.

Proposition 4.2.1. *Let $n \geq 1$. Then $\tilde{F}_n(\zeta)$ satisfies the recurrence relation*

$$\tilde{F}_{n+1}(\zeta) = \zeta - \frac{1}{\tilde{F}_n(\zeta)}, \quad \tilde{F}_1(\zeta) = \zeta. \quad (4.27)$$

Proof. Consider the recurrence relation (2.35). Then for $n = 1$

$$\tilde{F}_1(\zeta) = \frac{F_1(\zeta)}{F_0(\zeta)} = \zeta.$$

For $n \geq 2$, dividing the last equation of (2.35) by $F_{j-1}(\zeta)$ we arrive at (4.27). \square

One can see that functions \tilde{F}_n and G_n are related to each other in the following manner.

Proposition 4.2.2. *Let $\xi \in \mathbb{C} \setminus \{0\}$ and $n \geq 1$. Then*

$$G_n(\xi) = \tilde{F}_n\left(\xi + \frac{1}{\xi}\right). \quad (4.28)$$

Proof. We proceed by induction. For $n = 1$, we have

$$G_1(\xi) = \frac{\xi^2 - \xi^{-2}}{\xi - \xi^{-1}} = \xi + \frac{1}{\xi} = \tilde{F}_1\left(\xi + \frac{1}{\xi}\right)$$

so (4.28) holds for $n = 1$. Now assume that (4.28) is true for some $n \in \mathbb{N}$. Then

$$\begin{aligned} G_{n+1}(\xi) &= \frac{\xi^{n+2} - \xi^{-n-2}}{\xi^{n+1} - \xi^{-n-1}} \\ &= \frac{(\xi^{n+1} - \xi^{-n-1})(\xi - \xi^{-1}) - \xi^n + \xi^{-n}}{\xi^{n+1} - \xi^{-n-1}} \\ &= \xi + \xi^{-1} - \frac{1}{G_n(\xi)} = \tilde{F}_{n+1}\left(\xi + \frac{1}{\xi}\right). \end{aligned}$$

Thus, by induction, (4.28) holds for all $n \in \mathbb{N}$. \square

Using Proposition 4.2.1, the characteristic equation (4.5) can be reformulated in terms of \tilde{F}_n as follows.

Corollary 4.2.3. *Let λ, σ, τ be related by (3.6), let $\mathbf{u}, \mathbf{v}, \sigma, \tau$ solve (4.1)-(4.2), and let $\sigma, \tau \notin \{\mu_n, \dots, \mu_1\}$. Then $\lambda = (\sigma + \tau)/2$ is a simple eigenvalue of \mathcal{A}_c , and*

$$\tilde{F}_n(\sigma)\tilde{F}_n(\tau) = -1. \quad (4.29)$$

The equation (4.29) can also be deduced from Theorem 4.1.7 and Proposition 4.2.2. We now verify the reformulation of Conjecture 1.3.3 given as in Theorem 1.3.4(iii).

Proof of Theorem 1.3.4(iii). Let λ, σ, τ be related by (3.6). Then, by Corollary 4.2.3, λ is a non-real eigenvalue of \mathcal{A}_c if and only if $\sigma, \tau \in \mathbb{C} \setminus \mathbb{R}$ satisfy (4.29). We have by (3.6) that $\text{Im}(\lambda) = \text{Im}(\sigma) = \text{Im}(\tau)$. Moreover, by Lemma 3.1.3 we have the symmetry $\lambda \rightarrow \bar{\lambda}$, which implies $\sigma \rightarrow \bar{\sigma}$ and $\tau \rightarrow \bar{\tau}$. Therefore it is sufficient to consider the non-real solutions of (4.29) with $\text{Im}(\sigma) = \text{Im}(\tau) > 0$. \square

We omit the proof of part (ii) since its reformulation is immediate by (4.26).

It is easy to see that if $|\sigma| \geq 2$ and $|\tau| \geq 2$, then there is no such $(\sigma, \tau) \in \mathbb{C}^2$ which satisfies (4.29). This is due to the following lemma.

Lemma 4.2.4. *If $|\zeta| \geq 2$, then $|\tilde{F}_n(\zeta)| > 1$ for all $n \geq 1$.*

Proof. We proceed by induction. For $n = 1$, the statement is obvious. Now assume that $|\tilde{F}_n(\zeta)| > 1$ holds for some $n \in \mathbb{N}$. Then

$$\left| \zeta - \frac{1}{|\tilde{F}_n(\zeta)|} \right| \leq \left| \zeta - \frac{1}{\tilde{F}_n(\zeta)} \right| = |\tilde{F}_{n+1}(\zeta)|.$$

Since $|\zeta| \geq 2$ and $\frac{1}{|\tilde{F}_n(\zeta)|} < 1$, the left-hand side of the inequality is greater than one, and therefore $|\tilde{F}_{n+1}(\zeta)| > 1$. Then, by induction, the statement holds for all $n \in \mathbb{N}$. \square

Using the three term recurrence relation (4.27), the function \tilde{F}_n can be written in a continued fraction expansion

$$\tilde{F}_n(\zeta) = \zeta - \frac{1}{\zeta - \frac{1}{\dots - \frac{1}{\zeta}}}$$

However, the main problem in here is that ζ is a complex number. In addition, since the functions $\tilde{F}_n(\zeta)$ can be expressed in terms of the ratios of Chebyshev polynomials of the second kind, we can treat Conjecture 1.3.3 as a ratio of orthogonal polynomials. In Section 4.5.2, we will apply the ratio asymptotics, which were mentioned in Section 2.3.4, and obtain some bounds on the function $\tilde{F}_n(\zeta)$.

4.2.2 The area between $|z| = 1$ and $|z \pm i|^2 < 2$

In Section 4.1.2, we used the change of variables (4.8) to re-write the characteristic equation in terms of z and w , as in Lemma 4.1.7(a) and (c). Therefore another way of expressing Conjecture 1.3.3 is looking at the equivalent statements of λ in terms of z and w , which was stated in the introduction. Our goal in this subsection is to prove and clarify Theorem 1.3.4(iv). We will then give some numerical examples to support this result. We will illustrate z and w values correspond to the non-real eigenvalues of \mathcal{A}_c on the same complex plane. We also give the Gershgorin-type localisation result and its illustration in Section 4.5.3.3.

Remark 4.2.5. The characteristic equation of the pencil problem for non-real eigenvalues was given in Theorem 4.1.7(c). In fact, the equation (4.15) holds also for the real eigenvalues of \mathcal{A}_c as long as $z^n \neq z^{-n}$ and $w^n \neq w^{-n}$. This is due to Theorem 4.1.7(a), and that

$$\frac{f_n(z, w)}{(z^n - z^{-n})(w^n - w^{-n})} = G_n(z)G_n(w) - 1.$$

It is also easy to see that if λ is non-real, then by Theorem 4.1.7(b), we have $z^n \neq z^{-n}$ and $w^n \neq w^{-n}$.

A direct calculation leads to the following auxiliary result.

Lemma 4.2.6. *The roots of $|z + 1/z| = 2$ are exactly $z = \pm i + \sqrt{2}e^{i\varphi}$ where $\varphi \in [0, 2\pi]$, and therefore*

$$\left|z + \frac{1}{z}\right| < 2 \Leftrightarrow |z \pm i| < \sqrt{2}. \quad (4.30)$$

We can now clarify the reformulation of Conjecture 1.3.3 in terms of corresponding z and w .

Proof of Theorem 1.3.4(iv). Recall that if λ is a non-real eigenvalue of the pencil \mathcal{A}_c , we then define z, w to be the unique solutions of (4.9) and (4.10), respectively, which satisfy $|z| > 1$ and $|w| > 1$. Then by Theorem 4.1.7(b), λ is non-real if and only if $z, w \in \mathbb{C} \setminus \mathbb{R}$ with

$|z| > 1$ and $|w| > 1$. By Lemma 4.2.6, we can re-write the statement of the conjecture as any solutions z, w of (4.15) should lie in the set $\mathcal{Z}_1 \cup \mathcal{Z}_2$ where

$$\mathcal{Z}_1 = \mathcal{D}(i, \sqrt{2}) \setminus \overline{\mathcal{D}}(0, 1), \quad \mathcal{Z}_2 = \mathcal{D}(-i, \sqrt{2}) \setminus \overline{\mathcal{D}}(0, 1),$$

where $\overline{\mathcal{D}}(o, r)$ denotes the closure of the disk $\mathcal{D}(o, r)$. □

We present some numerical experiments in Figure 4.2. For simplicity, we omit the values of z and w which lie on the unit circle $\partial\mathcal{D}(0, 1)$ and on the real line. It is clear from (4.18)-(4.20) that these values correspond to the real eigenvalues of \mathcal{A}_c . We take the set of non-real eigenvalues in the λ -plane and plot them in a different complex plane using (4.8). We superimpose corresponding values of z and w in the same complex plane by solving the quadratic equations (4.9) and (4.10) on a finely spaced grid of c values. The black dashed circle represents the unit circle $\partial\mathcal{D}(0, 1)$, the orange circle represents $\partial\mathcal{D}(i, \sqrt{2})$ and the light-orange shaded area represents the set \mathcal{Z}_1 . The green circle represents $\partial\mathcal{D}(-i, \sqrt{2})$ and the light-green shaded area represents the set \mathcal{Z}_2 . The red and blue curves, which correspond to values of z and w respectively, are exactly the non-real eigenvalue curves of the pencil \mathcal{A}_c under the change of variables (4.8). For presentation purposes, in the four illustrations we zoom in on an area near the unit circle.

In Figure 4.2 we illustrate all non-real eigenvalue curves, however we would like to know only whether (1.19) is satisfied. Without seeing the dynamics, it is difficult to understand which two values (z and w) correspond to the same c . The only thing we know from Remark 4.1.8 is that $\text{Im}\lambda > 0$ implies $\text{Im}(z) > 0$ and $\text{Im}(w) > 0$. According to the figure, the eigenvalues (in terms of z and w) always appear from the unit circle and disappear to the unit circle. Conjecture 1.3.3 will be broken if one eigenvalue escapes from the unit circle and then travels to the real axis. In this case, it would have to cross the forbidden region. The important thing in this figure is that they do not cross the boundary of \mathcal{Z}_1 and \mathcal{Z}_2 . Conjecture 1.3.3 appear to be true since whatever escapes from the unit circle, returns to the unit circle without going through the forbidden area. Hence, both z and w , which correspond to the non-real eigenvalues, seem to lie in $\mathcal{Z}_1 \cup \mathcal{Z}_2$.

4.2.3 Intersection of Gershgorin disks

Recall that $\mathcal{G}(A)$ represents the Gershgorin set of A . Our main aim was to enhance the Gershgorin Theorem when applied to the non-real eigenvalues of the pencil \mathcal{A}_c (or the non-self-adjoint matrix \mathbf{A}_c), but we could not. In this section, we apply the Gershgorin Theorem to our problem. In Section 4.5.3, we will discuss the application of known Gershgorin-type results mentioned in Section 2.2 to our problem in more detail.

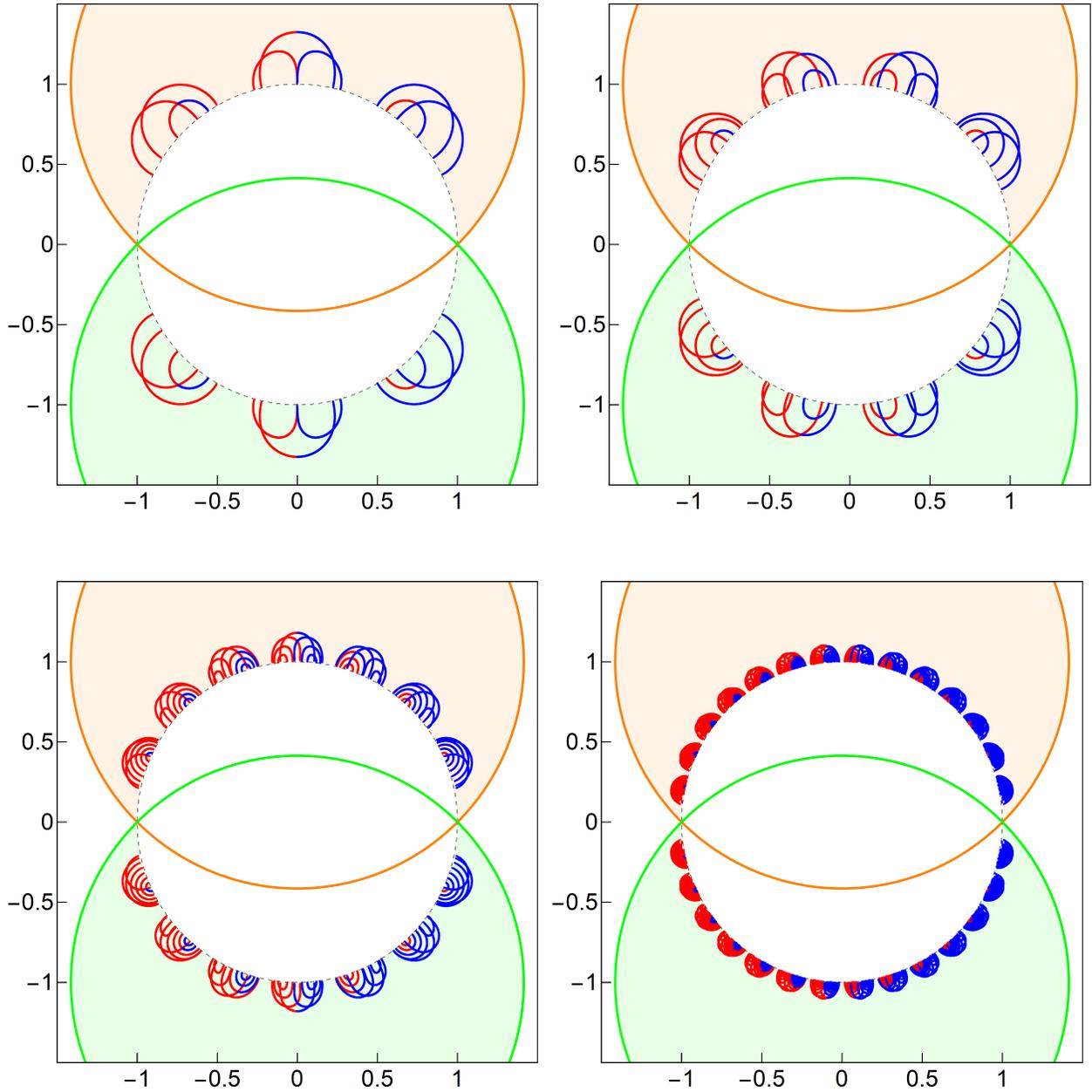


Figure 4.2: \mathcal{Z}_1 (orange dashed region), $\partial\mathcal{D}(i, \sqrt{2})$ (orange circle), \mathcal{Z}_2 (green dashed region), $\partial\mathcal{D}(-i, \sqrt{2})$ (green circle), $\partial\mathcal{D}(0, 1)$ (black dashed circle), drawn in the complex plane, together with the superimposition of z (red curves) and w (blue curves) values, which correspond to the non-real eigenvalues only, for c values between 0 and 2 with step-size of 10^{-3} . Left top: $n = 3$. Right top: $n = 4$. Left bottom: $n = 7$. Right bottom: $n = 14$.

The Gershgorin set $\mathcal{G}(\mathbf{A}_c)$ consists of four different disks defined by

$$\begin{aligned} \mathcal{G}_1(\mathbf{A}_c) &= \overline{\mathcal{D}}(c, 1), & \mathcal{G}_i(\mathbf{A}_c) &= \overline{\mathcal{D}}(c, 2), \\ \mathcal{G}_j(\mathbf{A}_c) &= \overline{\mathcal{D}}(-c, 2), & \mathcal{G}_{2n}(\mathbf{A}_c) &= \overline{\mathcal{D}}(-c, 1) \end{aligned}$$

where $i = 2, \dots, n$ and $j = n + 1, \dots, N - 1$. Then $\mathcal{G}_1(\mathbf{A}_c) \subset \mathcal{G}_i(\mathbf{A}_c)$ and $\mathcal{G}_{2n}(\mathbf{A}_c) \subset \mathcal{G}_j(\mathbf{A}_c)$, and therefore

$$\bigcup_{i=1}^n \mathcal{G}_i(\mathbf{A}_c) = \overline{\mathcal{D}}(c, 2), \quad \bigcup_{j=n+1}^{2n} \mathcal{G}_j(\mathbf{A}_c) = \overline{\mathcal{D}}(-c, 2).$$

Hence, we obtain

$$\text{Spec}(\mathbf{A}_c) \subseteq \mathcal{G}(\mathbf{A}_c) = \overline{\mathcal{D}}(c, 2) \cup \overline{\mathcal{D}}(-c, 2).$$

We illustrate the union in Figure 4.3.

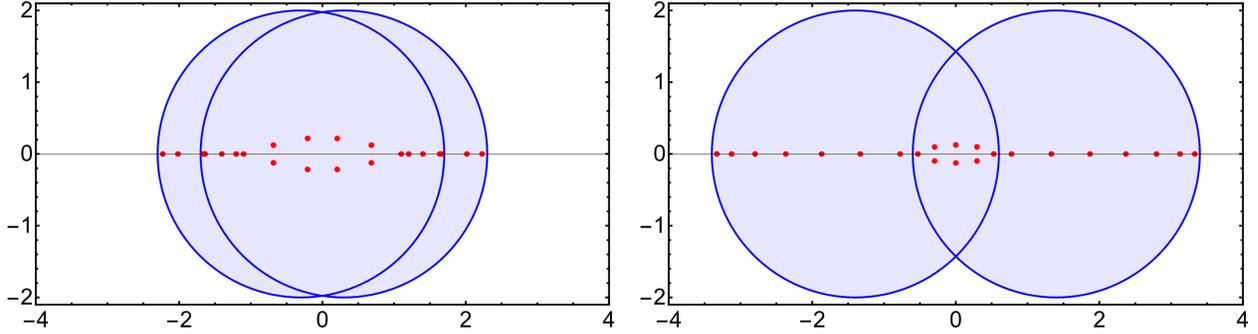


Figure 4.3: For $n = 11$, red dots represent the eigenvalues of \mathbf{A}_c and the blue shaded region is the Gershgorin set $\mathcal{G}(\mathbf{A}_c)$, i.e. the union $\overline{\mathcal{D}}(c, 2) \cup \overline{\mathcal{D}}(-c, 2)$. The boundaries of each disk are represented by the blue circles. Left: $c = 0.3$. Right: $c = 1.4$.

However, when we focus on the non-real eigenvalues of \mathbf{A}_c , we observe that they all seem to lie in the intersection of the Gershgorin disks. Note that

$$\mathcal{D}(c, 2) \cap \mathcal{D}(-c, 2) = \{\lambda \in \mathbb{C} : |\lambda - c| < 2 \text{ and } |\lambda + c| < 2\}.$$

Then this leads us to another reformulation of the conjecture as in Theorem 1.3.4(v), i.e. if $\lambda \in \text{Spec}(\mathbf{A}_c) \setminus \mathbb{R}$, then $\lambda \in \mathcal{D}(c, 2) \cap \mathcal{D}(-c, 2)$.

As shown in Section 2.2, there exists no Gershgorin-type localisation result which gives a bound only for the non-real eigenvalues of a matrix. All existing results give a bound for the whole spectrum of a matrix. In this case, we see that Conjecture 1.3.3 is somewhat stronger than Gershgorin Theorem. Unfortunately, we could not obtain any such region which contains only the non-real spectrum of \mathbf{A}_c . Nevertheless, we have the following result.

Lemma 4.2.7. *Conjecture 1.3.3 is satisfied for those $\lambda \in \text{Spec}(\mathbf{A}_c) \setminus \mathbb{R}$ for which $|\sigma| = |\tau|$ with λ, σ, τ related by (3.6).*

Proof. The case $|\sigma| = |\tau|$ implies that

$$|\lambda - c| = |\lambda + c| \Leftrightarrow c = 0 \text{ or } \operatorname{Re}(\lambda) = 0,$$

i.e. λ is equidistant from both c and $-c$. In other words, these eigenvalues lie on the imaginary axis in the complex plane. Since the Gershgorin disks $\overline{D}(c, 2)$ and $\overline{D}(-c, 2)$ are symmetric with respect to the imaginary axis, the intersection as well as the union of two Gershgorin disks always cover the imaginary axis by Gershgorin Theorem. Therefore these purely imaginary eigenvalues always lie in the intersection of two Gershgorin disks which implies that both $|\sigma| = |\lambda - c|$ and $|\tau| = |\lambda + c|$ are smaller than two. Note that the boundaries does not play a role since the characteristic equation (4.29) is not satisfied by Lemma 4.2.4 if $|\sigma| = |\tau| = 2$. \square

4.3 Partial cases

The goal of this section is to prove that the Conjecture 1.3.3 holds for $n = 2$ and for $n = 3$. We will prove the equivalent statement of the conjecture given in Theorem 1.3.4(iii). The purpose of this section is to see that even for small size, the result is non-trivial, computations get messy and there is no pattern.

When $n = 1$, it is straightforward to see that Conjecture 1.3.3 is satisfied:

$$\sigma\tau = -1 \quad \Rightarrow \quad \tau = -\frac{1}{\sigma} = -\frac{\operatorname{Re}(\sigma) - i\operatorname{Im}(\sigma)}{|\sigma|^2}$$

and since $\operatorname{Im}(\sigma) = \operatorname{Im}(\tau)$, we obtain

$$\operatorname{Im}(\tau) = \frac{\operatorname{Im}(\sigma)}{|\sigma|^2} \quad \Rightarrow \quad |\sigma| = 1 \quad \Rightarrow \quad |\tau| = \frac{1}{|\sigma|} = 1,$$

as required.

Now, set

$$\sigma = x + iy, \quad \tau = t + iy, \tag{4.31}$$

where $x, t \in \mathbb{R}$ and $y \in \mathbb{R} \setminus \{0\}$, and look for solutions of the characteristic equation (4.29) when $n = 2$ and $n = 3$. We will see in each situation that there are two cases: either $|\sigma| = |\tau|$ or $|\sigma| \neq |\tau|$. We know by Lemma 4.2.7 that Conjecture 1.3.3 is satisfied in the case $|\sigma| = |\tau|$ for all $n \in \mathbb{N}$. Nevertheless, we emphasise that we will include the proof of this case for the sake of completeness. In addition, recall from Corollary 3.1.8 that $|y| \leq 1$.

4.3.1 The case $n = 2$

For $n = 2$, the equation becomes

$$\left(\sigma - \frac{1}{\sigma}\right) \left(\tau - \frac{1}{\tau}\right) = -1 \quad \Leftrightarrow \quad -\sigma\tau = (\sigma^2 - 1)(\tau^2 - 1),$$

substituting (4.31) into (4.29) gives

$$-(x + iy)(t + iy) = (x^2 - y^2 - 1 + i2xy)(t^2 - y^2 - 1 + i2ty).$$

Separating the real and imaginary parts of the equation gives the system of two equations

$$y^2 - xt = (x^2 - y^2 - 1)(t^2 - y^2 - 1) - 4xty^2, \quad (4.32)$$

$$-(xy + yt) = 2ty(x^2 - y^2 - 1) + 2xy(t^2 - y^2 - 1). \quad (4.33)$$

Re-arranging equation (4.33) gives

$$(x + t)(1 + 2y^2 - 2xt) = 0. \quad (4.34)$$

We now have two cases, either $t = -x$ or $1 + 2y^2 - 2xt = 0$.

The first case: $|\sigma| = |\tau|$

Let $t = -x$ which also implies that $|\sigma| = |\tau|$. Then using this in (4.32), we have, after simplification, that

$$4x^2 - 1 = (x^2 + y^2)^2 + (x^2 + y^2)$$

and since $4x^2 - 1 < 4|\sigma|^2 - 1$, the above equation reduces to

$$|\sigma|^4 + |\sigma|^2 < 4|\sigma|^2 - 1$$

which implies

$$\left(|\sigma|^2 - \frac{3}{2}\right)^2 - \frac{5}{4} < 0,$$

and so

$$\frac{3}{2} - \sqrt{\frac{5}{4}} < |\sigma|^2 < \frac{3}{2} + \sqrt{\frac{5}{4}},$$

and since $|\sigma| = |\tau|$, we obtain $|\sigma|, |\tau| < 2$.

The second case: $|\sigma| \neq |\tau|$

Take $t \neq -x$. Re-arranging (4.32), we have

$$\begin{aligned} 0 &= (x^2 - y^2 - 1)(t^2 - y^2 - 1) - 4xty^2 - y^2 + xt \\ &= x^2t^2 - x^2y^2 - x^2 - y^2t^2 + y^4 + y^2 - t^2 + y^2 + 1 - 4xty^2 - y^2 + xt \\ &= (xt)^2 + xt - y^2(x^2 + t^2) - (x^2 + t^2) + y^4 + y^2 + 1 - 4y^2(xt) \end{aligned}$$

Then using $xt = y^2 + 1/2$ into the above equation, we obtain

$$\begin{aligned} 0 &= (y^4 + y^2 + \frac{1}{4}) - (y^2 + 1)(x^2 + t^2) + y^4 + y^2 + 1 - 4y^4 - 2y^2 + y^2 + \frac{1}{2} \\ &= -(y^2 + 1)(x^2 + t^2) - 2y^4 + 1 + \frac{1}{4} + y^2 + \frac{1}{2} \\ &= -(y^2 + 1)(x^2 + t^2 + 2y^2) + 2y^4 + 2y^2 - 2y^4 + y^2 + \frac{7}{4} \\ &= -(y^2 + 1)(|\sigma|^2 + |\tau|^2) + 3y^2 + \frac{7}{4} \end{aligned}$$

which implies

$$|\sigma|^2 + |\tau|^2 = \frac{3y^2 + \frac{7}{4}}{y^2 + 1} = 3 - \frac{5}{4(y^2 + 1)} < 3$$

for all y . Thus, $|\sigma|, |\tau| < 2$. Hence the conjecture is true for $n = 2$.

4.3.2 The case $n = 3$

When $n = 3$, equation (4.29) becomes

$$\begin{aligned} \left(\sigma - \frac{1}{\sigma - \frac{1}{\sigma}}\right) \left(\tau - \frac{1}{\tau - \frac{1}{\tau}}\right) = -1 &\Leftrightarrow \left(\sigma - \frac{\sigma}{\sigma^2 - 1}\right) \left(\tau - \frac{\tau}{\tau^2 - 1}\right) = -1 \\ &\Leftrightarrow (\sigma^3 - 2\sigma)(\tau^3 - 2\tau) = -(\sigma^2 - 1)(\tau^2 - 1). \quad (4.35) \end{aligned}$$

First, re-arranging the imaginary part of LHS of (4.35), we have

$$\begin{aligned} &\text{Im}[(\sigma^3 - 2\sigma)(\tau^3 - 2\tau)] \\ &= \text{Im}[(x^3 - 3xy^2 - 2x + i(3x^2y - 2y - y^3))(t^3 - 3ty^2 - 2t + i(3t^2y - 2y - y^3))] \\ &= (x^3 - 3xy^2 - 2x)(3t^2y - 2y - y^3) + (t^3 - 3ty^2 - 2t)(3x^2y - 2y - y^3) \\ &= -x^3y^3 + 3x^3t^2y - 2x^3y + 3xy^5 - 9xt^2y^3 + 8xy^3 - 6xt^2y + 4xy \\ &\quad - t^3y^3 + 3x^2t^3y - 2t^3y + 3ty^5 - 9x^2ty^3 + 8ty^3 - 6x^2ty + 4ty \\ &= -y^3(x^3 + t^3) + 3x^2t^2y(x + t) - 2y(x^3 + t^3) + 3y^5(x + t) \end{aligned}$$

$$\begin{aligned}
& -9xty^3(x+t) + 8y^3(x+t) - 6xty(x+t) + 4y(x+t) \\
& = (x+t)y[(-y^2-2)(x^2+t^2-xt) + 3x^2t^2 + 3y^4 - 9xty^2 + 8y^2 - 6xt + 4], \quad (4.36)
\end{aligned}$$

and re-arranging the imaginary part of RHS of (4.35), we have

$$\begin{aligned}
\text{Im}[-(\sigma^2-1)(\tau^2-1)] &= \text{Im}[-(x^2-y^2-1+i2xy)(t^2-y^2-1+i2ty)] \\
&= -(2ty(x^2-y^2-1) + 2xy(t^2-y^2-1)) \\
&= -2y(tx^2-ty^2-t+xt^2-xy^2-x) \\
&= -2y[(x+t)(xt-y^2-1)]. \quad (4.37)
\end{aligned}$$

Equating (4.36) and (4.37) we obtain

$$(x+t)y[(-y^2-2)(x^2+t^2-xt) + 3x^2t^2 + 3y^4 - 9xty^2 + 6y^2 - 4xt + 2] = 0. \quad (4.38)$$

Since $y \neq 0$, we again have two cases; either $|\sigma| = |\tau|$ or $|\sigma| \neq |\tau|$.

The first case: $|\sigma| = |\tau|$

The first case; let $t = -x$, i.e. $|\sigma| = |\tau|$. Then from the real part of LHS of (4.35), we have

$$\begin{aligned}
& \text{Re}[(\sigma^3-2\sigma)(\tau^3-2\tau)] \\
&= \text{Re}[(x^3-3xy^2-2x+i(3x^2y-2y-y^3))(t^3-3ty^2-2t+i(3t^2y-2y-y^3))] \\
&= (x^3-3xy^2-2x)(t^3-3ty^2-2t) - (3x^2y-2y-y^3)(3t^2y-2y-y^3) \\
&= -(x^3-3xy^2-2x)^2 - (3x^2y-2y-y^3)^2 \\
&= -(x^6+3x^4y^2+3x^2y^4+y^6-4x^4+4x^2+4y^4+4y^2) \\
&= -[(x^2+y^2)^3-4x^4+4y^4+4(x^2+y^2)] \\
&= -|\sigma|^6-4|\sigma|^2+4x^4-4y^4 \\
&= -|\sigma|^6-4|\sigma|^2+4(x^2+y^2)^2-8x^2y^2-8y^4 \\
&= -|\sigma|^6-4|\sigma|^2+4|\sigma|^4-8y^2|\sigma|^2, \quad (4.39)
\end{aligned}$$

and from the real part of RHS of (4.35),

$$\begin{aligned}
\text{Re}[-(\sigma^2-1)(\tau^2-1)] &= \text{Re}[-(x^2-y^2-1+i2xy)(z^2-y^2-1+i2zy)] \\
&= -(x^2-y^2-1)(z^2-y^2-1) + 2xy2zy \\
&= -(x^4+y^4+1-2x^2y^2-2x^2+2y^2+4x^2y^2) \\
&= -[(x^2+y^2)^2-2x^2+2y^2+1] \\
&= -|\sigma|^4+2|\sigma|^2-4y^2-1. \quad (4.40)
\end{aligned}$$

Equating (4.39) and (4.40) yields

$$|\sigma|^6 - 5|\sigma|^4 + |\sigma|^2(6 + 8y^2) - 4y^2 - 1 = 0. \quad (4.41)$$

Let $s := |\sigma|^2$ and denote

$$\tilde{f}_y(s) := s^3 - 5s^2 + (6 + 8y^2)s - 4y^2 - 1,$$

then the equation (4.41) becomes

$$\tilde{f}_y(s) = 0.$$

We now need to show that if s_0 is a root of $\tilde{f}_y(s)$ for some $y > 0$, then $s_0 < 4$. First, note that when $s = 4$, the function is positive for all y , i.e.

$$\tilde{f}_y(4) = 7 + 28y^2 > 0.$$

Now, we want to show that the function is increasing for all $y > 0$ and $s > 4$. Taking the derivative with respect to s gives

$$\tilde{f}'_y(s) = 3s^2 - 10s + 6 + 8y^2.$$

$\tilde{f}'_y(s)$ is increasing in s for $s \geq 5/3$, therefore for $s \geq 4$,

$$\tilde{f}'_y(s) \geq \tilde{f}'_y(4) = 14 + 8y^2 > 0.$$

Thus, $\tilde{f}'_y(s) > 0$ for $s \geq 4$, and if there exists s_0 such that $\tilde{f}_y(s_0) = 0$, then $s_0 < 4$. Hence we prove that if $|\sigma| = |\tau|$, then $|\sigma|, |\tau| < 2$.

The second case: $|\sigma| \neq |\tau|$

The second case is to show if $|\sigma| \neq |\tau|$ then $|\sigma|, |\tau| < 2$. Proving this case is not as easy as the first case. We will see that all calculations get messy and the problem involves finding zeros of high degree polynomials.

Dividing (4.38) by $y(x + t)$ and re-arranging it gives

$$3x^2t^2 - 2xt(4y^2 + 1) - (x^2 + t^2)(y^2 + 2) + 3y^4 + 6y^2 + 2 = 0,$$

which implies

$$3x^2t^2 = 2xt(4y^2 + 1) + (|\sigma|^2 + |\tau|^2)(y^2 + 2) - 2y^4 - 4y^2 - 3y^4 - 6y^2 - 2.$$

Let $p := xt$ and $A := |\sigma|^2 + |\tau|^2$, then

$$3p^2 - p(8y^2 + 2) - A(y^2 + 2) + 5y^4 + 10y^2 + 2 = 0. \quad (4.42)$$

Now, the real part of (4.35), after simplification, is

$$\begin{aligned} x^3t^3 + x^2t^2(-9y^2 + 1) + xt(-(3y^2 + 2)(x^2 + t^2) + 9y^4 + 8y^2 + 4) \\ + (x^2 + t^2)(3y^4 + 5y^2 - 1) - y^6 - 3y^4 - 2y^2 + 1 = 0. \end{aligned}$$

Using $p = xt$ and $A = |\sigma|^2 + |\tau|^2$ yields

$$\begin{aligned} p^3 + p^2(-9y^2 + 1) + p(-A(3y^2 + 2) + 15y^4 + 12y^2 + 4) \\ + A(3y^4 + 5y^2 - 1) - 7y^6 - 13y^4 + 1 = 0. \end{aligned} \quad (4.43)$$

The equation (4.42) implies that

$$3p^2 = p(8y^2 + 2) + A(y^2 + 2) - (5y^4 + 10y^2 + 2). \quad (4.44)$$

Multiplying (4.44) by p and substituting this into (4.43) gives

$$\begin{aligned} p^2 \left(\frac{8y^2 + 2}{3} - 9y^2 + 1 \right) \\ + p \left(A \frac{y^2 + 2}{3} - \frac{5y^4 + 10y^2 + 2}{3} - A(3y^2 + 2) + 15y^4 + 12y^2 + 4 \right) \\ + A(3y^4 + 5y^2 - 1) - 7y^6 - 13y^4 + 1 = 0, \end{aligned}$$

which implies

$$\begin{aligned} p^2(-19y^2 + 5) + p(A(-8y^2 - 4) + 40y^4 + 26y^2 + 10) \\ + 3A(3y^4 + 5y^2 - 1) - 3(7y^6 + 13y^4 - 1) = 0. \end{aligned}$$

Substituting equation (4.44) into the above equation yields

$$\begin{aligned} (-19y^2 + 5) [p(8y^2 + 2) + A(y^2 + 2) - (5y^4 + 10y^2 + 2)] \\ + 3p(A(-8y^2 - 4) + 40y^4 + 26y^2 + 10) \\ + 9A(3y^4 + 5y^2 - 1) - 9(7y^6 + 13y^4 - 1) = 0, \end{aligned}$$

which implies

$$\begin{aligned} p((-19y^2 + 5)(8y^2 + 2) - 3A(8y^2 + 4) + 120y^4 + 78y^2 + 30) \\ + A((-19y^2 + 5)(y^2 + 2) + 27y^4 + 45y^2 - 9) \end{aligned}$$

$$+ (19y^2 - 5)(5y^4 + 10y^2 + 2) - 9(7y^6 + 13y^4 - 1) = 0,$$

and so

$$p(3A(8y^2 + 4) + 32y^4 - 80y^2 - 40) = A(8y^4 + 12y^2 + 1) + 32y^6 + 48y^4 - 12y^2 - 1.$$

Resolving the last equation with respect to p and substituting back into (4.42) gives

$$\begin{aligned} \widehat{f}_y(A) := & \frac{-144A^3(y^2 + 2)(2y^2 + 1)^2 + 9A^2(640y^6 + 1776y^4 + 1208y^2 + 243)}{16(A(6y^2 + 3) + 8y^4 - 20y^2 - 10)^2} \\ & - 9A \frac{(512y^8 + 3584y^6 + 6256y^4 + 3328y^2 + 558)}{16(A(6y^2 + 3) + 8y^4 - 20y^2 - 10)^2} \\ & + \frac{20736y^8 + 75456y^6 + 77328y^4 + 27432y^2 + 3123}{16(A(6y^2 + 3) + 8y^4 - 20y^2 - 10)^2} = 0. \end{aligned}$$

We want to show that if A_0 is a root of $\widehat{f}_y(A)$ for some $0 < y \leq 1$, then $A_0 < 4$. First, we show that $\widehat{f}_y(4)$ is negative for all $y \in (0, 1]$:

$$\widehat{f}_y(4) = \frac{9(256y^8 + 192y^6 - 304y^4 - 152y^2 - 45)}{64(4y^4 + 2y^2 + 1)^2}.$$

The denominator of $\widehat{f}_y(4)$ is positive. By using $y^8 < y^6 < y^4$ and $-y^2 < -y^4$ we obtain

$$\begin{aligned} 64(4y^4 + 2y^2 + 1)^2 \widehat{f}_y(4) &= 2304y^8 + 1728y^6 - 2736y^4 - 1368y^2 - 405 \\ &< 2304y^4 + 1728y^4 - 2736y^4 - 1368y^4 - 405 \\ &= -72y^4 - 405 < 0 \end{aligned}$$

which implies

$$\widehat{f}_y(4) < 0, \quad \forall y \in (0, 1]. \quad (4.45)$$

Second, taking the derivative with respect to A , we will show that $\widehat{f}_y(A)$ is decreasing for all $0 < y \leq 1$ and $A > 4$. A direct calculation gives

$$\widehat{f}'_y(A) = \frac{k_3 A^3 + k_2 A^2 + k_1 A + k_0}{k_{-1}},$$

where

$$\begin{aligned} k_3(y) &= -1728y^8 - 6048y^6 - 6480y^4 - 2808y^2 - 432, \\ k_2(y) &= -6912y^{10} - 3456y^8 + 44928y^6 + 61344y^4 + 28080y^2 + 4320, \\ k_1(y) &= 59904y^{10} + 116352y^8 - 73008y^6 - 185472y^4 - 92466y^2 - 14337, \\ k_0(y) &= -18432y^{12} - 207360y^{10} - 394560y^8 - 85824y^6 + 164376y^4 + 98946y^2 + 15741 \end{aligned}$$

$$k_{-1}(A, y) = 8(A(6y^2 + 3) + 8y^4 - 20y^2 - 10)^3.$$

It is easy to see that the denominator $k_{-1}(A, y)$ is always positive when $A > 4$, and therefore we will ignore it since it does not play a role to the sign of $\widehat{f}'_y(A)$. To understand the sign of the numerator of $\widehat{f}'_y(A)$, we need the following result.

Lemma 4.3.1. *For any $0 < y \leq 1$,*

(i) $4^3k_3 + 4^2k_2 + 4k_1 + k_0 < 0$.

(ii) $k_1 + k_2 + k_3 < 0$.

(iii) $k_1 + k_3 < 0$.

Proof.

(i) We have

$$\begin{aligned} 4^3k_3 + 4^2k_2 + 4k_1 + k_0 &= -18432y^{12} - 78336y^{10} - 95040y^8 - 46080y^6 - 10728y^4 \\ &\quad - 1350y^2 - 135 \end{aligned}$$

which is always negative.

(ii) We have

$$k_1 + k_2 + k_3 = 52992y^{10} + 111168y^8 - 34128y^6 - 130608y^4 - 67194y^2 - 10449.$$

By using $y^{10} < y^8 < y^4$ and $-y^2 < -y^4$, we obtain

$$\begin{aligned} k_1 + k_2 + k_3 &< 52992y^4 + 111168y^4 - 34128y^6 - 130608y^4 - 67194y^4 - 10449 \\ &= -34128y^6 - 33642y^4 - 10449 \end{aligned}$$

which is also negative.

(iii) We have

$$k_1 + k_3 = 59904y^{10} + 114624y^8 - 79056y^6 - 191952y^4 - 95274y^2 - 14769.$$

By using $y^{10} < y^8 < y^6$ and $-y^4 < -y^6$, we get

$$\begin{aligned} k_1 + k_3 &< 59904y^6 + 114624y^6 - 79056y^6 - 191952y^6 - 95274y^2 - 14769 \\ &= -96480y^6 - 95274y^2 - 14769 < 0 \end{aligned}$$

as required. □

Now, consider the numerator of $\widehat{f}_y(A)$. Using, consecutively, Lemma 4.3.1(i), (ii) and then (iii), we have

$$\begin{aligned}
k_3A^3 + k_2A^2 + k_1A + k_0 &< k_3(A^3 - 4^3) + k_2(A^2 - 4^2) + k_1(A - 4) \\
&< k_3(A^3 - 4^3 - A^2 + 4^2) + k_1(-A^2 + 4^2 + A - 4) \\
&< k_3(A^3 - 4^3 - A^2 + 4^2 + A^2 - 4^2 - A + 4) \\
&= k_3(A - 4)(A^2 + 4A + 15) < 0,
\end{aligned}$$

for all $0 < y \leq 1$ and all $A \geq 4$. Thus,

$$\widehat{f}_y(A) < 0 \quad \forall A \geq 4, \forall y \in (0, 1]. \quad (4.46)$$

Combining (4.45) and (4.46), we conclude that if there exists A_0 such that $\widehat{f}_y(A_0) = 0$, then $A_0 < 4$.

4.4 Formal asymptotic expansion as $c \rightarrow 0$

As we mentioned in Theorem 3.1.2, all eigenvalues of \mathcal{A}_0 (i.e. \mathcal{A}_c when $c = 0$) are non-real, and Davies and Levitin [19] determined the asymptotic behaviour of the eigenvalues of the pencil \mathcal{A}_c for large n . When c increases, each complex conjugate pair moves towards each other and meets on the real line. Numerical experiments show that eigenvalues move along a curve until each pair collide for the first time on the real line (see Level-1 in Table 5.1). Our aim in this section is to understand and describe the curve corresponding to the non-real eigenvalues of \mathcal{A}_c as c goes to zero. The investigation will be carried out by using a formal asymptotic expansion method.

Recall the substitution (4.8) and note that each non-real eigenvalue λ corresponds to one non-real z and one non-real w value, which lie outside of the unit disk. When $c = 0$, the relation (4.8) reduces to

$$\lambda_0 = z_0 + \frac{1}{z_0} = w_0 + \frac{1}{w_0}, \quad (4.47)$$

where λ_0 denotes the eigenvalues of \mathcal{A}_0 . In addition, $z_0, w_0 \in \mathbb{C} \setminus \mathbb{R}$ such that $|z_0|, |w_0| > 1$. Then, for simplicity, we can take $z_0 = w_0$. Therefore, when $c = 0$ the reduced characteristic equation (4.15) becomes

$$(G_n(z_0))^2 = -1 \quad \Rightarrow \quad G_n(z_0) = \pm i. \quad (4.48)$$

Davies and Levitin [19] found that as $n \rightarrow \infty$ any solutions of (4.48), which lie in the first quadrant, satisfy

$$z_0 = re^{i\theta}, \quad (4.49)$$

where

$$r = \left(\tan \left(\frac{\pi}{4} + \frac{\theta}{2} \right) \right)^{1/2n}, \quad \theta = \frac{2\pi k}{2n+1}, \quad k = 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor,$$

up to order $O(n^{-1})$. We then extend the result to the other quadrants by using symmetries described in Lemma 3.1.3 and the relation (4.47). If n is odd, there are additionally two purely z_0 values which satisfy

$$z_0 = \pm i \left(1 + \frac{\log(n)}{n} (1 + o(1)) \right). \quad (4.50)$$

The idea is to fix the size of matrix $n \in \mathbb{N}$ and seek a solution of the form of a power series in c , i.e.

$$\lambda = \lambda_0 + c\lambda_1 + c^2\lambda_2 + O(c^3), \quad (4.51)$$

$$z = z_0 + cz_1 + c^2z_2 + O(c^3), \quad (4.52)$$

$$w = w_0 + cw_1 + c^2w_2 + O(c^3). \quad (4.53)$$

We will then find $\lambda_1, \lambda_2, z_1, z_2, w_1, w_2$ in terms of z_0 . Afterwards, using the asymptotics for λ_0 and $z_0 = w_0$, i.e. (4.49), we will find an approximate solution to the behaviour of the eigenvalues of \mathcal{A}_c when c is small. We will mainly use the relation (4.8) and the characteristic equation (4.15).

Before stating our main result, we introduce some functions. Let $\zeta \in \mathbb{C}$, then define

$$g_n = g_n(\zeta) := \zeta^n + \zeta^{-n}, \quad (4.54)$$

$$b_n = b_n(\zeta) := \zeta^n - \zeta^{-n}, \quad (4.55)$$

$$Q_n(\zeta) = \frac{(n+1)g_{n+1} - ng_n G_n(\zeta)}{\zeta b_n}, \quad (4.56)$$

$$\widehat{Q}_n(\zeta) = \zeta^{-2} \left(G_n(\zeta) \left(n \frac{\zeta^n}{b_n} + n^2 \frac{g_n^2}{b_n^2} \right) - \frac{n+1}{b_n} \left(\zeta^{-n-1} + n \frac{g_n g_{n+1}}{b_n} \right) \right). \quad (4.57)$$

Our main result in this section is the following.

Theorem 4.4.1. *Let $\lambda_0 \notin \mathbb{R}$ be an eigenvalue of \mathcal{A}_0 , let z_0 be the unique solution of (4.47) outside the unit disk. Then there is an eigenvalue λ of \mathcal{A}_c such that*

$$\lambda = z_0 + \frac{1}{z_0} + c^2 \left(\frac{z_0^2}{2(z_0^2 - 1)} \left(\frac{Q_n^2(z_0) - 2G_n(z_0)\widehat{Q}_n(z_0)}{G_n(z_0)Q_n(z_0)} \right) + \frac{z_0}{(z_0^2 - 1)^2} \right) + O(c^3), \quad (4.58)$$

and moreover

$$z = z_0 + c \left(\frac{z_0^2}{1 - z_0^2} \right) + c^2 \left(\frac{z_0^4}{2(z_0^2 - 1)^2} \left(\frac{Q_n^2(z_0) - 2G_n(z_0)\widehat{Q}_n(z_0)}{G_n(z_0)Q_n(z_0)} \right) \right) + O(c^3),$$

$$w = z_0 - c \left(\frac{z_0^2}{1 - z_0^2} \right) + c^2 \left(\frac{z_0^4}{2(z_0^2 - 1)^2} \left(\frac{Q_n^2(z_0) - 2G_n(z_0)\widehat{Q}_n(z_0)}{G_n(z_0)Q_n(z_0)} \right) \right) + O(c^3),$$

where λ, z, w are related by (4.8).

Remark 4.4.2. Combining (4.58) and (4.51), we can easily deduce that $\lambda_1 = 0$, thus the perturbation of eigenvalues is quadratic in c . Note that our asymptotic procedure uses the fact that the eigenvalues are simple. Therefore the results will not work after the first collisions, because when we have a double eigenvalue, the characteristic equation is no longer an analytic function of a parameter, and therefore we cannot expand it into a series.

Before proving the result, we start with some numerical experiments. The results are illustrated in the $(\operatorname{Re}\lambda, 2n\operatorname{Im}\lambda)$ -plane in Figure 4.4, and in terms of z and w values in the complex plane in Figure 4.5. We know that all eigenvalues of \mathcal{A}_c are non-real when $c = 0$. As c increases, the figures show that our asymptotics catch the eigenvalues until they become real for the first time (or until z and w hit the unit circle for the first time). We can see that our asymptotics, as expected, do not catch the eigenvalues after they become real. The corresponding z and w values move along the unit circle whereas the asymptotic expansion that we found keep moving as c increases.

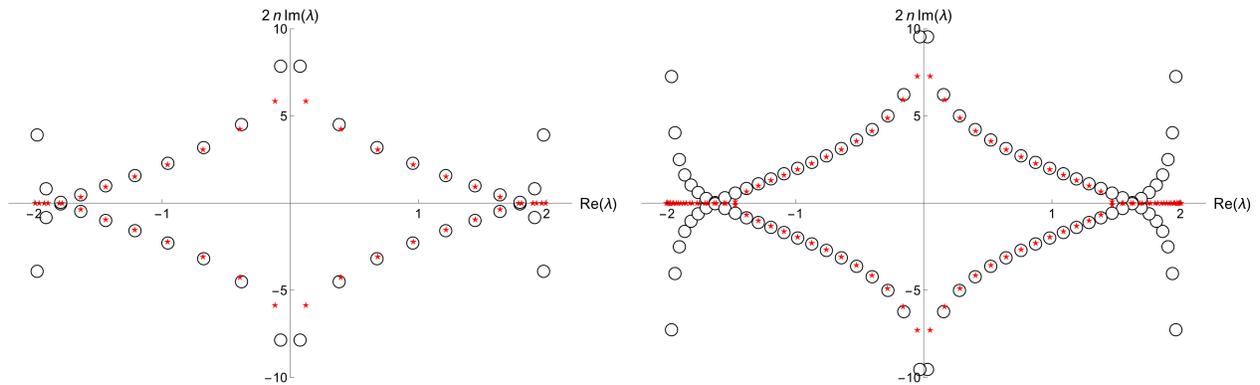


Figure 4.4: $\operatorname{Spec}(\mathcal{A}_c)$ in the $(\operatorname{Re}\lambda, 2n\operatorname{Im}\lambda)$ -plane with λ values (red stars) and their asymptotic values (white circles) given by Theorem 4.4.1. Left: for $n = 20$ and $c = 0.015$. Right: for $n = 50$ and $c = 0.01$.

In order to prove Theorem 4.4.1, we need some auxiliary results. The next result provides a formula which converts a ratio of two polynomials to a geometric series.

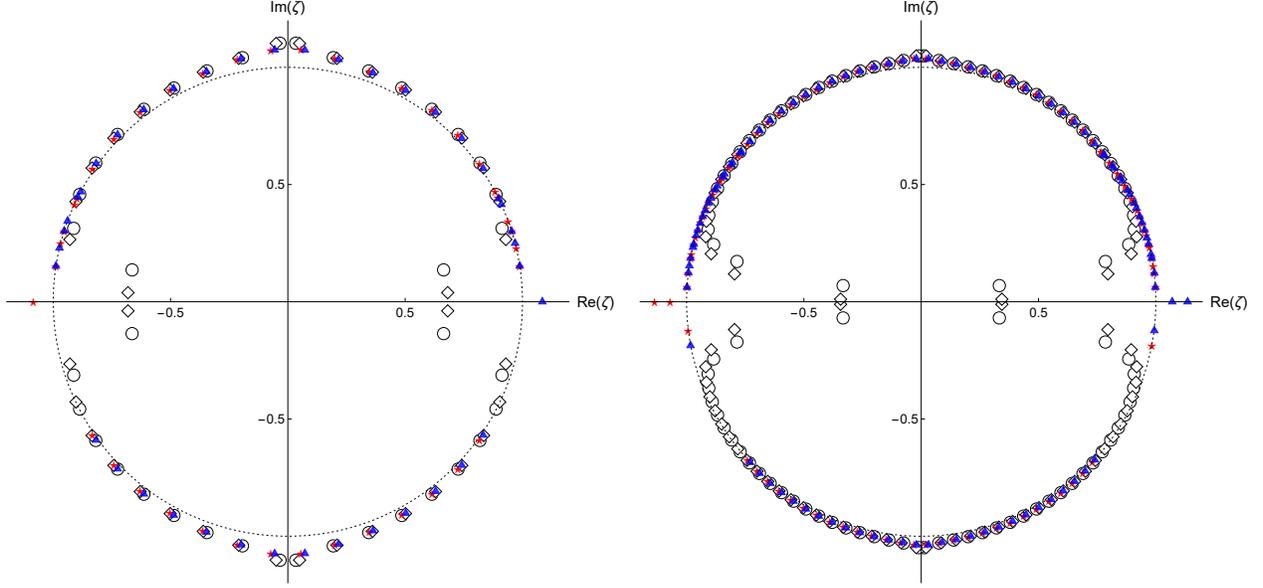


Figure 4.5: $\text{Spec}(\mathcal{A}_c)$ in the complex plane with z values (red stars), w values (blue triangles), asymptotic values of z (white circles), asymptotic values of w (white diamonds), the unit circle $\partial D(0, 1)$ (dotted circle). Left: for $n = 20$ and $c = 0.015$. Right: for $n = 50$ and $c = 0.01$.

Lemma 4.4.3. Let $a, b, \gamma, \delta, \rho, \phi \in \mathbb{C}$. As $c \rightarrow 0$,

$$\frac{a + c\gamma + c^2\rho}{b + c\delta + c^2\phi} = \frac{a}{b} + c \left(\frac{\gamma}{b} - a \frac{\delta}{b^2} \right) + c^2 \left(\frac{\rho}{b} - \frac{\gamma\delta + a\phi}{b^2} + \frac{a\delta^2}{b^3} \right) + O(c^3).$$

Proof. As $c \rightarrow 0$, expanding the ratio as a geometric series up to terms of order $O(c^3)$ gives

$$\begin{aligned} \frac{a + c\gamma + c^2\rho}{b + c\delta + c^2\phi} &= \frac{a + c\gamma + c^2\rho}{b} \left(\frac{1}{1 + c\frac{\delta}{b} + c^2\frac{\phi}{b}} \right) + O(c^3) \\ &= \frac{a + c\gamma + c^2\rho}{b} \left(1 - c\frac{\delta}{b} - c^2\frac{\phi}{b} + \left(c\frac{\delta}{b} + c^2\frac{\phi}{b} \right)^2 \right) + O(c^3) \\ &= \frac{a + c\gamma + c^2\rho}{b} \left(1 - c\frac{\delta}{b} + c^2 \left(\frac{\delta^2}{b^2} - \frac{\phi}{b} \right) \right) + O(c^3) \\ &= (a + c\gamma + c^2\rho) \left(\frac{1}{b} - \frac{\delta}{b^2}c + c^2 \left(\frac{\delta^2}{b^3} - \frac{\phi}{b^2} \right) \right) + O(c^3) \\ &= \frac{a}{b} + c \left(\frac{\gamma}{b} - a \frac{\delta}{b^2} \right) + c^2 \left(\frac{\rho}{b} - \frac{\gamma\delta + a\phi}{b^2} + \frac{a\delta^2}{b^3} \right) + O(c^3). \end{aligned}$$

□

In the next result, we derive an asymptotic expansion for the function $G_n(z)$ by using Lemma 4.4.3.

Lemma 4.4.4. *Suppose that $c \rightarrow 0$, and $z = z_0 + cz_1 + c^2z_2 + O(c^3)$. Then*

$$G_n(z) = G_n(z_0) + cz_1Q_n(z_0) + c^2 \left(z_2Q_n(z_0) + z_1^2\widehat{Q}_n(z_0) \right) + O(c^3),$$

where the functions Q_n, \widehat{Q}_n depend only z_0 and are as given in (4.56)-(4.57).

Proof. Substituting the asymptotic expansion (4.52) into the function $G_n(z)$ we have

$$\begin{aligned} G_n(z) &= G_n(z_0 + cz_1 + c^2z_2 + O(c^3)) \\ &= \frac{(z_0 + cz_1 + c^2z_2)^{n+1} - (z_0 + cz_1 + c^2z_2)^{-n-1}}{(z_0 + cz_1 + c^2z_2)^n - (z_0 + cz_1 + c^2z_2)^{-n}} + O(c^3). \end{aligned} \quad (4.59)$$

Now, calculating each power separately we get

$$z^{n+1} = (z_0 + cz_1 + c^2z_2)^{n+1} = z_0^{n+1} + c(n+1)z_0^n z_1 + c^2(n+1)z_0^{n-1} \left(z_0 z_2 + \frac{n}{2} z_1^2 \right) + O(c^3)$$

and

$$\begin{aligned} z^{-n-1} &= (z^{n+1})^{-1} = \left(z_0^{n+1} + c(n+1)z_0^n z_1 + c^2(n+1)z_0^{n-1} \left(z_0 z_2 + \frac{n}{2} z_1^2 \right) \right)^{-1} + O(c^3) \\ &= z_0^{-n-1} \left(1 + c(n+1) \frac{z_1}{z_0} + c^2(n+1) \left(\frac{z_2}{z_0} + \frac{n}{2} \frac{z_1^2}{z_0^2} \right) \right)^{-1} + O(c^3) \\ &= z_0^{-n-1} \left(1 - c(n+1) \frac{z_1}{z_0} - c^2(n+1) \left(\frac{z_2}{z_0} + \frac{n}{2} \frac{z_1^2}{z_0^2} \right) + c^2(n+1)^2 \frac{z_1^2}{z_0^2} \right) + O(c^3) \\ &= z_0^{-n-1} \left(1 - c(n+1) \frac{z_1}{z_0} - c^2(n+1) \left(\frac{z_2}{z_0} - \left(\frac{n}{2} + 1 \right) \frac{z_1^2}{z_0^2} \right) \right) + O(c^3) \\ &= z_0^{-n-1} - c(n+1) \frac{z_1}{z_0^{n+2}} - c^2(n+1) \left(\frac{z_2}{z_0^{n+2}} - \left(\frac{n}{2} + 1 \right) \frac{z_1^2}{z_0^{n+3}} \right) + O(c^3) \end{aligned}$$

Similarly,

$$\begin{aligned} z^n &= z_0^n + cnz_0^{n-1}z_1 + c^2nz_0^{n-2} \left(z_0 z_2 + \frac{n-1}{2} z_1^2 \right) + O(c^3) \\ z^{-n} &= z_0^{-n} - cn \frac{z_1}{z_0^{n+1}} - c^2n \left(\frac{z_2}{z_0^{n+1}} - \left(\frac{n+1}{2} \right) \frac{z_1^2}{z_0^{n+2}} \right) + O(c^3). \end{aligned}$$

Then

$$\begin{aligned} z^{n+1} - z^{-n-1} &= z_0^{n+1} - z_0^{-n-1} + c(n+1)z_1(z_0^n + z_0^{-n-2}) \\ &\quad + c^2(n+1) \left(z_2(z_0^n + z_0^{-n-2}) + z_1^2 z_0^{-2} \frac{n}{2} (z_0^{n+1} - z_0^{-n-1}) - z_1^2 z_0^{-n-3} \right) + O(c^3), \end{aligned} \quad (4.60)$$

and

$$z^n - z^{-n} = z_0^n - z_0^{-n} + cnz_1(z_0^{n-1} + z_0^{-n-1})$$

$$+ c^2 n \left(z_2 (z_0^{n-1} + z_0^{-n-1}) + z_1^2 z_0^{-2} \frac{n-1}{2} (z_0^n - z_0^{-n}) - z_1^2 z_0^{-n-2} \right) + O(c^3). \quad (4.61)$$

Substituting (4.60) and (4.61) into the function (4.59), we have a ratio of two polynomials in c of degree 2. Therefore we will apply to Lemma 4.4.3 so as to write the function G_n as a polynomial in c . The complex constants in Lemma 4.4.3 can be matched as

$$\begin{aligned} a &= z_0^{n+1} - z_0^{-n-1}, \\ b &= b_n = z_0^n - z_0^{-n}, \\ \gamma &= (n+1)z_1 z_0^{-1} g_{n+1}, \\ \delta &= n z_1 z_0^{-1} g_n, \\ \rho &= (n+1) \left(z_2 z_0^{-1} g_{n+1} + \frac{n}{2} z_1^2 z_0^{-2} (z_0^{n+1} - z_0^{-n-1}) - z_1^2 z_0^{-n-3} \right), \\ \phi &= n \left(z_2 z_0^{-1} g_n + \frac{n-1}{2} z_1^2 z_0^{-2} (z_0^n - z_0^{-n}) - z_1^2 z_0^{-n-2} \right). \end{aligned}$$

Then applying Lemma 4.4.3 gives, at order $O(c^0)$,

$$\frac{a}{b} = \frac{z_0^{n+1} - z_0^{-n-1}}{z_0^n - z_0^{-n}} = G_n(z_0),$$

and at order $O(c^1)$,

$$\frac{\gamma}{b} - \frac{a\delta}{b^2} = z_1 \left(\frac{(n+1)z_0^{-1} g_{n+1} - n z_0^{-1} g_n G_n(z_0)}{z_0^n - z_0^{-n}} \right) = z_1 Q_n(z_0).$$

To find the coefficient of c^2 in (4.59), we have

$$\frac{\rho}{b} - \frac{\gamma\delta + a\phi}{b^2} + \frac{a\delta^2}{b^3} = \frac{\rho}{b} - \frac{\gamma\delta}{b^2} - \frac{\phi}{b} G_n(z_0) + \frac{\delta^2}{b^2} G_n(z_0).$$

Then at order $O(c^2)$,

$$\begin{aligned} &(n+1) \left(z_2 z_0^{-1} \frac{g_{n+1}}{b_n} + \frac{n}{2} z_1^2 z_0^{-2} G_n(z_0) - \frac{z_1^2 z_0^{-n-3}}{b_n} \right) - n(n+1) z_1^2 z_0^{-2} \frac{g_n g_{n+1}}{b_n} \\ &- n G_n(z_0) \left(z_2 z_0^{-1} \frac{g_n}{b_n} + \left(\frac{n-1}{2} \right) z_1^2 z_0^{-2} - \frac{z_1^2 z_0^{-n-2}}{b_n} \right) + n^2 G_n(z_0) z_1^2 z_0^{-2} \frac{g_n^2}{b_n^2} \end{aligned}$$

which can be simplified to

$$z_2 Q_n(z_0) + z_1^2 \widehat{Q}_n(z_0),$$

as required. □

The next result will be helpful when determining the terms at order $O(c)$.

Lemma 4.4.5. *Suppose $z \in \mathbb{C} \setminus \mathbb{R}$ such that $|z| > 1$ and $G_n^2(z) = -1$. Then $Q_n(z) \neq 0$.*

Proof. Suppose that $\exists z \in \mathbb{C} \setminus \mathbb{R}$ such that $G_n^2(z) = -1$ and $Q_n(z) = 0$. We have

$$G_n^2(z) = \frac{z^{2n+2} + z^{-2n-2} - 2}{z^{2n} + z^{-2n} - 2} = -1 \Leftrightarrow z^{2n+2} + z^{-2n-2} = -z^{2n} - z^{-2n} + 4.$$

Then

$$\begin{aligned} Q_n(z) = 0 &\Leftrightarrow (n+1)(z^{n+1} + z^{-n-1}) = n(z^n + z^{-n})G_n(z) \\ &\Rightarrow (n+1)^2(z^{2n+2} + z^{-2n-2} + 2) = n^2(z^{2n} + z^{-2n} + 2)(-1) \\ &\Leftrightarrow (n^2 + 2n + 1)(-z^{2n} - z^{-2n} + 6) = -n^2(z^{2n} + z^{-2n} + 2). \end{aligned}$$

Now let $t = z^{2n} + z^{-2n}$. Then

$$\begin{aligned} (n^2 + 2n + 1)(-t + 6) = -n^2(t + 2) &\Leftrightarrow 6n^2 - n^2t + 12n - 2nt + 6 - t = -n^2t - 2n^2 \\ &\Leftrightarrow 8n^2 + 12n + 6 = t(2n + 1). \end{aligned}$$

Looking at the imaginary parts of the last equation, we deduce that

$$\text{Im}(t) = 0 \Leftrightarrow \text{Im}(z^{2n} + z^{-2n}) = 0 \Leftrightarrow \text{Im}(z^{2n}) = -\text{Im}\left(\frac{1}{z^{2n}}\right) = \frac{\text{Im}(z^{2n})}{|z^{2n}|^2} \Leftrightarrow |z|^{4n} = 1.$$

Therefore, if $\exists z$ such that $G_n^2(z) = -1$ and $Q_n(z) = 0$, then $|z| = 1$ which is a contradiction. \square

We can now prove our main result.

Proof of Theorem 4.4.1. First, recall that z_0 and w_0 correspond to the eigenvalues of \mathcal{A}_0 which are all non-real and $|z_0|, |w_0| > 1$. Also, we take $z_0 = w_0$. Note that the functions Q_n, \widehat{Q}_n depend only on z_0 and therefore, we have from Lemma 4.4.4 that

$$G_n(z) = G_n(z_0) + cz_1 Q_n(z_0) + c^2 \left(z_2 Q_n(z_0) + z_1^2 \widehat{Q}_n(z_0) \right) + O(c^3), \quad (4.62)$$

and

$$G_n(w) = G_n(z_0) + cw_1 Q_n(z_0) + c^2 \left(w_2 Q_n(z_0) + w_1^2 \widehat{Q}_n(z_0) \right) + O(c^3). \quad (4.63)$$

Then substituting (4.62) and (4.63) into the characteristic equation (4.15), and then equating powers of c , we find at order $O(c^0)$ that

$$(G_n(z_0))^2 = -1 \Rightarrow G_n(z_0) = \pm i.$$

Note that $Q_n(z_0) \neq 0$ by Conjecture 4.4.5, then we have at order $O(c^1)$ that

$$(z_1 + w_1)Q_n(z_0)G_n(z_0) = 0 \quad \Rightarrow \quad w_1 = -z_1,$$

and at order $O(c^2)$ that

$$(z_2 + w_2)G_n(z_0)Q_n(z_0) + 2z_1^2G_n(z_0)\widehat{Q}_n(z_0) - z_1^2Q_n^2(z_0) = 0. \quad (4.64)$$

Now, recall equation (4.8):

$$\lambda = z + \frac{1}{z} + c = w + \frac{1}{w} - c$$

Expanding $z + 1/z$ we have

$$z + \frac{1}{z} = z_0 + cz_1 + c^2z_2 + \frac{1}{z_0 + cz_1 + c^2z_2} + O(c^3) \quad (4.65)$$

$$= z_0 + cz_1 + c^2z_2 + \frac{1}{z_0} \left(\frac{1}{1 + c\frac{z_1}{z_0} + c^2\frac{z_2}{z_0^2}} \right) + O(c^3)$$

$$= z_0 + cz_1 + c^2z_2 + \frac{1}{z_0} \left(1 - c\frac{z_1}{z_0} - c^2\frac{z_2}{z_0^2} + \left(c\frac{z_1}{z_0} + c^2\frac{z_2}{z_0^2} \right)^2 \right) + O(c^3)$$

$$= z_0 + \frac{1}{z_0} + cz_1 \left(1 - \frac{1}{z_0^2} \right) + c^2 \left(z_2 \left(1 - \frac{1}{z_0^2} \right) + \frac{z_1^2}{z_0^3} \right) + O(c^3). \quad (4.66)$$

Similarly,

$$w + \frac{1}{w} = w_0 + \frac{1}{w_0} + cw_1 \left(1 - \frac{1}{w_0^2} \right) + c^2 \left(w_2 \left(1 - \frac{1}{w_0^2} \right) + \frac{w_1^2}{w_0^3} \right) + O(c^3). \quad (4.67)$$

Substituting the asymptotic expansions (4.66) and (4.67) into (4.8), and equating terms at each order we have at order $O(c^0)$ that

$$\lambda_0 = z_0 + \frac{1}{z_0} = w_0 + \frac{1}{w_0}$$

and we take $w_0 = z_0$. At order $O(c^1)$ we get

$$\lambda_1 = z_1 \left(1 - \frac{1}{z_0^2} \right) + 1 = w_1 \left(1 - \frac{1}{w_0^2} \right) - 1 \quad \Rightarrow \quad \lambda_1 = \frac{z_1 + w_1}{2} \left(1 - \frac{1}{z_0^2} \right) = 0,$$

which also implies

$$w_1 = -z_1 = \frac{z_0^2}{z_0^2 - 1}. \quad (4.68)$$

We have at order $O(c^2)$ that

$$\lambda_2 = z_2 \left(1 - \frac{1}{z_0^2} \right) + \frac{z_1^2}{z_0^3} = w_2 \left(1 - \frac{1}{w_0^2} \right) + \frac{w_1^2}{w_0^3} \quad \Rightarrow \quad z_2 = w_2. \quad (4.69)$$

Now, substituting $w_1 = -z_1$ and $w_2 = z_2$ into (4.64) gives

$$2z_2G_n(z_0)Q_n(z_0) = z_1^2 \left(Q_n^2(z_0) - 2G_n(z_0)\widehat{Q}_n(z_0) \right),$$

then substituting (4.68) into above, we can write z_2 in terms of z_0 as

$$z_2 = \frac{z_0^4}{2(z_0^2 - 1)^2} \left(\frac{Q_n^2(z_0) - 2G_n(z_0)\widehat{Q}_n(z_0)}{G_n(z_0)Q_n(z_0)} \right).$$

Now substituting z_1 and z_2 into (4.69), we find λ_2 in terms of z_0 as

$$\lambda_2 = \frac{z_0^2}{2(z_0^2 - 1)} \left(\frac{Q_n^2(z_0) - 2G_n(z_0)\widehat{Q}_n(z_0)}{G_n(z_0)Q_n(z_0)} \right) + \frac{z_0}{(z_0^2 - 1)^2}.$$

□

4.5 Improved bounds and ways to bound

4.5.1 Block-structure estimates

In this section, we apply Theorem 2.1.6 to our problem immediately. Take $\mathbf{X} = S^{-1}H_c^{(2n)}$. First, remark that Theorem 2.1.6 is most informative if $\delta = |\langle A_{12}\mathbf{v}, \mathbf{u} \rangle|$ is very small, which can happen even if $\|A_{12}\|$ is not small. Moreover, $|\operatorname{Im}\lambda| \leq |b|$ by Lemma 2.1.1, and Davies and Levitin [19] showed that one cannot hope for a result better than $|b| = |\langle A_{12}\mathbf{v}, \mathbf{u} \rangle| = O(1/N)$, and that even this is only possible if $|\operatorname{Re}\lambda|$ is not too close to 0. Proving such a bound depends on using the explicit expressions for \mathbf{u} , \mathbf{v} and A_{12} .

Now, take $A_{11} = H_0 + cI$, $A_{22} = -H_0 - cI$, and the dimension of \mathbf{X} is $N = 2n$. Recall that the eigenvalues μ_j of H_0 are as given in (2.37). Then

$$a_1 = \mu_n + c = 2 \cos\left(\frac{\pi n}{n+1}\right) + c = -2 \cos\left(\frac{\pi}{n+1}\right) + c = -2 + c + \epsilon,$$

and similarly

$$a_2 = \mu_1 + c = 2 \cos\left(\frac{\pi}{n+1}\right) = 2 + c - \epsilon,$$

$$d_1 = -2 \cos\left(\frac{\pi}{n+1}\right) - c = -2 - c + \epsilon,$$

$$d_2 = -2 \cos\left(\frac{\pi n}{n+1}\right) - c = 2 - c - \epsilon.$$

In all these formulae

$$\epsilon := 2 - \mu_1 = 2 - 2 \cos\left(\frac{\pi}{n+1}\right) = O(n^{-2}).$$

The inequality of Theorem 2.1.6 reads then

$$-2 + c + \epsilon - \delta \leq \operatorname{Re} \lambda \leq 2 - c - \epsilon + \delta.$$

As we want to prove (in the "real parts" version of the conjecture as opposed to the possibly harder "modulus" version)

$$-2 + c \leq \operatorname{Re} \lambda \leq 2 - c,$$

the comparison shows that we actually need a bound $\delta = |\langle A_{12} \mathbf{v}, \mathbf{u} \rangle| \leq \epsilon = O(n^{-2})$ (and for all n , not just asymptotically) which is very difficult, by the remark in the beginning of this subsection without additional careful analysis.

4.5.2 Bounds on the ratios of Chebyshev polynomials of the second kind

The behaviour of the ratio for orthogonal polynomials of finite index is still an open question. As mentioned in Section 2.3.4, there exists a function for the limit on the ratio which is given by Simon [66]. However, we will show in this section that Simon's estimate when applied to our particular problem is not enough to prove the conjecture. In this section, we wish to provide a better understanding of the asymptotic behaviour on the finite ratios of the orthogonal polynomials since Simon's estimate is not sufficient.

Recall that the functions $\tilde{F}_n(\zeta)$, defined by (4.26), equal the ratio of Chebyshev polynomials of the second kind, i.e.

$$\tilde{F}_n(\zeta) = \frac{U_n(\zeta/2)}{U_{n-1}(\zeta/2)},$$

where $\zeta \in \mathbb{C} \setminus \operatorname{Spec} \left(H_0^{(n-1)} \right)$. In Corollary 4.2.3, we wrote the characteristic equation of the pencil \mathcal{A}_c in terms of \tilde{F}_n . We start the investigation by applying Theorem 2.3.8 to our particular problem.

Lemma 4.5.1. *Let $\sigma, \tau \in \mathbb{C} \setminus [-2, 2]$. Then*

$$\lim_{n \rightarrow \infty} \left[\tilde{F}_n(\sigma) \tilde{F}_n(\tau) \right] = -1 \Rightarrow \sigma = -\tau,$$

which implies $\lambda = 0$.

Proof. Using the formula (2.51), we have

$$\lim_{n \rightarrow \infty} \left[\tilde{F}_n(\sigma) \tilde{F}_n(\tau) \right] = \lim_{n \rightarrow \infty} \tilde{F}_n(\sigma) \lim_{n \rightarrow \infty} \tilde{F}_n(\tau) = -1$$

$$\begin{aligned}
&\Leftrightarrow \frac{1}{2}(\sigma + \sqrt{\sigma^2 - 4})\frac{1}{2}(\tau + \sqrt{\tau^2 - 4}) = -1 \\
&\Leftrightarrow (\sigma + \sqrt{\sigma^2 - 4})(\tau + \sqrt{\tau^2 - 4}) = -4.
\end{aligned} \tag{4.70}$$

Note that $(\tau + \sqrt{\tau^2 - 4})(\tau - \sqrt{\tau^2 - 4}) = 4$, then using this in (4.70) yields

$$\begin{aligned}
&\sigma + \sqrt{\sigma^2 - 4} = \sqrt{\tau^2 - 4} - \tau, \\
\Rightarrow &\sigma + \tau = \sqrt{\tau^2 - 4} - \sqrt{\sigma^2 - 4}, \\
\Rightarrow &\sigma^2 + \tau^2 + 2\sigma\tau = \tau^2 - 4 + \sigma^2 - 4 - 2\sqrt{(\sigma^2 - 4)(\tau^2 - 4)}, \\
\Rightarrow &\sigma\tau + 4 = -\sqrt{(\sigma^2 - 4)(\tau^2 - 4)}, \\
\Rightarrow &\sigma^2\tau^2 + 16 + 8\sigma\tau = \sigma^2\tau^2 + 16 - 4(\sigma^2 + \tau^2), \\
\Rightarrow &4(\sigma^2 + \tau^2) + 8\sigma\tau = 0, \\
\Rightarrow &4(\sigma + \tau)^2 = 0, \\
\Rightarrow &\sigma = -\tau,
\end{aligned}$$

as required. □

Remark 4.5.2. Note that the formula (2.51) does not depend on n . Indeed, Davies and Levitin [19] showed that the spectrum of the pencil \mathcal{A}_c converge to the real line as n tends to infinity.

Unfortunately, Proposition 2.3.10 does not give us much information either. Using part (i), we deduce the next two result.

Corollary 4.5.3. *For all $\zeta \in \mathbb{C}$, we have*

$$\left| \widetilde{F}_n(\zeta) \right| \geq \min_j \left| \zeta - \mu_j^{(n)} \right|. \tag{4.71}$$

Proof. Taking the absolute value of the equation (2.52) that

$$\begin{aligned}
\left| \frac{1}{\widetilde{F}_n(\zeta)} \right| &\leq \sum_{j=1}^n \left| \frac{\alpha_j^{(n)}}{\zeta - \mu_j^{(n)}} \right| \\
&\leq \frac{\sum_{j=1}^n \alpha_j^{(n)}}{\min_j |\zeta - \mu_j^{(n)}|} \\
&\leq \frac{1}{\min_j |\zeta - \mu_j^{(n)}|},
\end{aligned}$$

as required. □

Corollary 4.5.4. For all $\zeta \in \mathbb{C}$, we have

$$\left| \tilde{F}_n(\zeta) - \zeta \right| \leq \frac{1}{\min_k \left| \zeta - \mu_k^{(n-1)} \right|}.$$

Proof. We have

$$\tilde{F}_n(\zeta) = \frac{\prod_{j=1}^n (\zeta - \mu_j^{(n)})}{\prod_{k=1}^{n-1} (\zeta - \mu_k^{(n-1)})},$$

then doing long divisions of polynomials

$$\begin{aligned} \tilde{F}_n(\zeta) = \zeta + \sum_{k=1}^{n-1} \frac{a_k^{(n-1)}}{\zeta - \mu_k^{(n-1)}} &\Rightarrow \left| \tilde{F}_n(\zeta) - \zeta \right| \leq \sum_{k=1}^{n-1} \left| \frac{a_k^{(n-1)}}{\zeta - \mu_k^{(n-1)}} \right|, \\ &\leq \frac{\sum_{k=1}^{n-1} \left| a_k^{(n-1)} \right|}{\min_k \left| \zeta - \mu_k^{(n-1)} \right|}, \\ &= \frac{1}{\min_k \left| \zeta - \mu_k^{(n-1)} \right|} \end{aligned}$$

as required. □

Proposition 2.3.10(ii) tells us if $\text{Im}\zeta > 0$, then

$$\frac{\text{Im}\tilde{F}_n(\zeta)}{\left| \tilde{F}_n(\zeta) \right|} \leq \frac{1}{\text{Im}\zeta}.$$

Part (iii), which was $\text{Im}\zeta \leq \text{Im}\tilde{F}_n(\zeta)$, will be shown in Lemma 4.5.5(ii). We see that the results given in Section 2.3.4 do not give anything new for our case.

Now, we want to investigate the finite ratios of the Chebyshev polynomials of the second kind, i.e. the function \tilde{F}_n , in more detail. The general idea is to obtain better estimates for the function \tilde{F}_n , not only as the size n of the matrix $H_0^{(n)}$ goes to infinity but also for finite size matrix. We obtain various new inequalities. The following collection of lemmas reveals sharper estimates on some areas for the finite ratio of orthogonal polynomials and/or the moduli of the real part $\left| \text{Re} \left(\tilde{F}_n \right) \right|$. The original purpose of these inequalities was to obtain a contradiction to the case that one of $|\sigma|$ and $|\tau|$ can be greater than two. We have obtained many inequalities, however we failed to obtain a contradiction. The main problem is that we cannot introduce the condition $\text{Im}(\sigma) = \text{Im}(\tau)$ easily. Nonetheless, we still believe that they are new and useful bounds. The results up to the end of this subsection are joint with Sabine Bögli (unpublished).

Before stating the results, first recall from the basic properties of complex numbers that

$$\left| \tilde{F}_n(\zeta) \right| = \left| \zeta - \frac{1}{\tilde{F}_{n-1}(\zeta)} \right| \geq |\zeta| - \frac{1}{\left| \tilde{F}_{n-1}(\zeta) \right|}. \quad (4.72)$$

We now list several bounds related with the function \tilde{F}_n . In all results in this section, we always assume that $\zeta \in \mathbb{C} \setminus \text{Spec} \left(H_0^{(n-1)} \right)$.

Lemma 4.5.5.

- (i) If $\text{Im}\zeta > 0$, then $\text{Im}\tilde{F}_n(\zeta) > \text{Im}\zeta > 0$ for all $n \geq 2$.
- (ii) If $|\zeta| > 2$ and $\text{Re}\zeta > 0$, then $0 < \text{Re}\tilde{F}_n(\zeta) < \text{Re}\zeta$ for all $n \geq 2$.
- (iii) If $|\zeta| > 2$ and $\text{Re}\zeta < 0$, then $\text{Re}\tilde{F}_n(\zeta) < \text{Re}\zeta < 0$ for all $n \geq 2$.

Proof.

- (i) Let $\text{Im}\zeta > 0$. Then we have for $n = 2$ that

$$\text{Im}\tilde{F}_2(\zeta) = \text{Im}\zeta + \frac{\text{Im}\zeta}{|\zeta|^2} > \text{Im}\zeta,$$

so (i) holds for $n = 2$. Now assume that (i) is true for some $n \in \mathbb{N}$, i.e. $\text{Im}\tilde{F}_n(\zeta) > \text{Im}\zeta$. Then

$$\text{Im}\tilde{F}_{n+1}(\zeta) = \text{Im}\zeta + \frac{\text{Im}\tilde{F}_n(\zeta)}{\left| \tilde{F}_n(\zeta) \right|^2} > \text{Im}\zeta + \frac{\text{Im}\zeta}{\left| \tilde{F}_n(\zeta) \right|^2} > \text{Im}\zeta.$$

Then, by induction, (i) holds for all $n \geq 2$.

- (ii) Let $|\zeta| > 2$ and $\text{Re}\zeta > 0$. Then we have for $n = 2$ that

$$\text{Re}\tilde{F}_2(\zeta) = \text{Re}\zeta - \frac{\text{Re}\bar{\zeta}}{|\zeta|^2} = \text{Re}\zeta \left(1 - \frac{1}{|\zeta|^2} \right) < \text{Re}\zeta$$

so (ii) is true for $n = 2$. Now assume that the inequality holds for some $n \in \mathbb{N}$ and consider $n + 1$;

$$\text{Re}\tilde{F}_{n+1}(\zeta) = \text{Re}\zeta - \frac{\text{Re}\tilde{F}_n(\zeta)}{\left| \tilde{F}_n(\zeta) \right|^2} < \text{Re}\zeta,$$

since $0 < \text{Re}\tilde{F}_n(\zeta)$. Thus, by induction, (ii) holds for all $n \in \mathbb{N}$.

- (iii) The proof follows in a similar way to part (ii). □

The next result gives a bound on the moduli of the function $\tilde{F}_n(\zeta)$ without assuming any condition on ζ .

Lemma 4.5.6. For all $n \in \mathbb{N}$ and all $\zeta \in \mathbb{C} \setminus \text{Spec}(H_0^{(n)})$, the function $\tilde{F}_n(\zeta)$ satisfies

$$\left| \tilde{F}_n(\zeta) \right| \geq \tilde{F}_n(|\zeta|). \quad (4.73)$$

Proof. For $n = 1$, (4.73) is trivial. For $n = 2$, we have

$$\left| \tilde{F}_2(\zeta) \right| = \left| \zeta - \frac{1}{\tilde{F}_1(\zeta)} \right| = \left| \zeta - \frac{1}{\zeta} \right| \geq |\zeta| - \frac{1}{|\zeta|} = \tilde{F}_2(|\zeta|),$$

so (4.73) holds for $n = 2$. Now assume (4.73) holds for some $n \in \mathbb{N}$ and consider $n + 1$;

$$\begin{aligned} \left| \tilde{F}_{n+1}(\zeta) \right| &= \left| \zeta - \frac{1}{\tilde{F}_n(\zeta)} \right| \geq |\zeta| - \frac{1}{\left| \tilde{F}_n(\zeta) \right|} \\ &\geq |\zeta| - \frac{1}{\tilde{F}_n(|\zeta|)} \\ &= \tilde{F}_{n+1}(|\zeta|), \end{aligned}$$

i.e. (4.73) holds with n replaced by $n + 1$. By induction (4.73) holds for all $n \in \mathbb{N}$. \square

The next result gives monotonicity of the function $\tilde{F}_n(\zeta)$ on the real line.

Lemma 4.5.7. For every $n \in \mathbb{N}$, $\tilde{F}_n(\zeta)$ is a strictly increasing function on each real interval $(\mu_{j-1}^{(n-1)}, \mu_j^{(n-1)})$, $j = 1, \dots, n$, where we set $\mu_0^{(n-1)} := -\infty$ and $\mu_n^{(n-1)} := +\infty$.

Proof. First, it can be seen from the definition of \tilde{F}_n that the zeros of $\tilde{F}_n(\zeta)$ occur at the zeros of $F_n(\zeta)$, which are $\zeta = \mu_j^{(n)}$, and $\tilde{F}_n(\zeta)$ is a continuous function except at the zeros of $\tilde{F}_{n-1}(\zeta)$, which are $\zeta = \mu_k^{(n-1)}$.

Now, it is easy to see that for $n = 1$, $\tilde{F}_1(\zeta) = \zeta$ is strictly increasing on $(-\infty, \infty)$. For $n = 2$,

$$\tilde{F}_2(\zeta) = \zeta - \frac{1}{\zeta},$$

which is strictly increasing as z increases on $(-\infty, 0)$ and $(0, \infty)$, and blow-up occurs when $\tilde{F}_1(\zeta) = \zeta = 0$. Suppose that for $n \in \mathbb{N}$, $\tilde{F}_n(\zeta)$ is strictly increasing function except at the zeros of F_{n-1} , then $-1/\tilde{F}_n(\zeta)$ is strictly increasing function except at the zeros of $F_n(\zeta)$. Using $\tilde{F}_{n+1}(\zeta) = \zeta - 1/\tilde{F}_n(\zeta)$, we have that $\tilde{F}_{n+1}(\zeta)$ is strictly increasing function except at the zeros of $F_n(\zeta)$. Then the result follows. \square

We show in the next result that, for some values of $|\zeta|$, we can actually calculate the precise values of the function $\tilde{F}_n(|\zeta|)$.

Lemma 4.5.8. For each $n \in \mathbb{N}$, we have

$$\tilde{F}_n(2) = 1 + \frac{1}{n}. \quad (4.74)$$

Proof. For $n = 1$, we have $\tilde{F}_1(2) = 2$ and for $n = 2$, we have $\tilde{F}_2(2) = 2 - 1/2 = 3/2 = 1 + 1/2$ so (4.74) holds. Suppose (4.74) holds for some $n \in \mathbb{N}$. Then

$$\tilde{F}_{n+1}(2) = 2 - \frac{1}{\tilde{F}_n(2)} = 2 - \frac{1}{1 + \frac{1}{n}} = 2 - \frac{n}{n+1} = \frac{n+2}{n+1} = 1 + \frac{1}{n+1},$$

i.e. (4.74) holds with n replaced by $n + 1$. By induction (4.74) holds for all $n \in \mathbb{N}$. \square

Now, using Lemma 4.5.6, Lemma 4.5.7 and Lemma 4.5.8, we deduce two bounds on the moduli of $\tilde{F}_n(\zeta)$.

Corollary 4.5.9. We have for all $n \in \mathbb{N}$ and all $|\zeta| > 2$ that

$$\left| \tilde{F}_n(\zeta) \right| > 1 + \frac{1}{n}. \quad (4.75)$$

Proof. It immediately follows from Lemma 4.5.6, Lemma 4.5.7 and Lemma 4.5.8 that

$$\left| \tilde{F}_n(\zeta) \right| \geq \tilde{F}_n(|\zeta|) > \tilde{F}_n(2) = 1 + \frac{1}{n}.$$

\square

Lemma 4.5.10. For all $n \in \mathbb{N}$ and $|\zeta| > 2$, we have

$$\left| \tilde{F}_n(\zeta) \right| > |\zeta| - 1 + \frac{1}{n}. \quad (4.76)$$

Proof. Using (4.72) and Corollary 4.5.9, we have

$$\begin{aligned} \left| \tilde{F}_n(\zeta) \right| &\geq |\zeta| - \frac{1}{\left| \tilde{F}_{n-1}(\zeta) \right|} \\ &> |\zeta| - \frac{1}{\tilde{F}_{n-1}(2)} \\ &= |\zeta| - \frac{1}{1 + \frac{1}{n-1}} \\ &= |\zeta| - \frac{n-1}{n} \\ &= |\zeta| - 1 + \frac{1}{n}, \end{aligned}$$

as required. \square

Using Lemma 4.5.10, we deduce an enclosure for the moduli of $\tilde{F}_n(\zeta)$.

Lemma 4.5.11. *For all $n \in \mathbb{N}$ and $|\zeta| > 2$, we have*

$$\left| |\tilde{F}_n(\zeta)| - |\zeta| \right| < \frac{1}{|\zeta| - 1 + \frac{1}{n-1}}. \quad (4.77)$$

Proof. Using equation (4.72) and Lemma 4.5.10 together, we have for $|\zeta| > 2$:

$$\left| \tilde{F}_n(\zeta) \right| \geq |\zeta| - \frac{1}{\left| \tilde{F}_{n-1}(\zeta) \right|} > |\zeta| - \frac{1}{|\zeta| - 1 + \frac{1}{n-1}}. \quad (4.78)$$

On the other hand, we have

$$\begin{aligned} \left| \tilde{F}_n(\zeta) \right| - |\zeta| &= \left| \zeta - \frac{1}{\tilde{F}_{n-1}(\zeta)} \right| - |\zeta| \\ &\leq |\zeta| + \left| \frac{1}{\tilde{F}_{n-1}(\zeta)} \right| - |\zeta| \\ &= \frac{1}{\left| \tilde{F}_{n-1}(\zeta) \right|} \\ &< \frac{1}{|\zeta| - 1 + \frac{1}{n-1}}, \end{aligned} \quad (4.79)$$

where we used Lemma 4.5.10 to obtain the last inequality. Combining (4.78) and (4.79) we arrive at (4.77). \square

Next, we prove an enclosure for the imaginary part of $\tilde{F}_n(\zeta)$.

Lemma 4.5.12. *Assume that $\text{Im}\zeta > 0$. Then we have for all $n \in \mathbb{N}$ and $\zeta \in \mathbb{C}$ that*

$$\text{Im}\zeta \leq \text{Im} \left(\tilde{F}_n(\zeta) \right) < \text{Im}\zeta + 1 \quad (4.80)$$

with equality only for $n = 1$.

Proof. For the lower bound, we showed in Lemma 4.5.5(i) that $\text{Im}\zeta < \text{Im} \left(\tilde{F}_n(\zeta) \right)$ for all $n \geq 2$. In addition, the equality holds clearly only for $n = 1$. For the upper bound, we have

$$\begin{aligned} \text{Im} \left(\tilde{F}_n(\zeta) \right) &= \text{Im}\zeta - \text{Im} \left(\frac{1}{\tilde{F}_{n-1}(\zeta)} \right), \\ &= \text{Im}\zeta + \frac{\text{Im} \left(\tilde{F}_{n-1}(\zeta) \right)}{\left| \tilde{F}_{n-1}(\zeta) \right|^2} \\ &\leq \text{Im}\zeta + 1. \end{aligned}$$

\square

The following easy result gives a bound on the imaginary part of $\tilde{F}_n(\zeta)$.

Corollary 4.5.13. *If $|\zeta| > 2$, then for all $n \in \mathbb{N}$, we have*

$$\operatorname{Im} \left(\tilde{F}_n(\zeta) \right) < \operatorname{Im} \zeta + \frac{\operatorname{Im} \left(\tilde{F}_{n-1}(\zeta) \right)}{|\zeta| - 1 + \frac{1}{n-1}}$$

Proof. Using Lemma 4.5.10 we have

$$\operatorname{Im} \left(\tilde{F}_n(\zeta) \right) = \operatorname{Im} \zeta + \frac{\operatorname{Im} \left(\tilde{F}_{n-1}(\zeta) \right)}{\left| \tilde{F}_{n-1}(\zeta) \right|^2} \leq \operatorname{Im} \zeta + \frac{\operatorname{Im} \left(\tilde{F}_{n-1}(\zeta) \right)}{|\zeta| - 1 + \frac{1}{n-1}}.$$

□

Now, we prove an enclosure on the real part of $\tilde{F}_n(\zeta)$.

Lemma 4.5.14. *If $|\zeta| > 2$, then*

$$\left| \operatorname{Re} \left(\tilde{F}_n(\zeta) \right) - \operatorname{Re} \zeta \right| < \left(|\zeta| - 1 + \frac{1}{n-1} \right)^{-1} < 1.$$

Proof. Using Lemma 4.5.10 we have

$$\left| \operatorname{Re} \left(\tilde{F}_n(\zeta) \right) - \operatorname{Re} \zeta \right| = \left| \operatorname{Re} \left(\frac{1}{\tilde{F}_{n-1}(\zeta)} \right) \right| < \frac{1}{\left| \tilde{F}_{n-1}(\zeta) \right|} < \left(|\zeta| - 1 + \frac{1}{n-1} \right)^{-1} < 1.$$

□

Now, we give a bound on the moduli and on the real part of the function $\tilde{F}_n(\zeta)$ assuming the real part of the parameter ζ is greater than two.

Lemma 4.5.15. *If $|\operatorname{Re} \zeta| > 2$, then*

$$\left| \tilde{F}_n(\zeta) \right| > \sqrt{4 + (\operatorname{Im} \zeta)^2} - \frac{n-1}{n} > 1. \quad (4.81)$$

Proof. Using equation (4.78) and $|\operatorname{Re}(z)| > 2$, we obtain

$$\left| \tilde{F}_n(\zeta) \right| > \sqrt{4 + (\operatorname{Im} \zeta)^2} - \frac{1}{\sqrt{4 + (\operatorname{Im} \zeta)^2} - 1 + \frac{1}{n-1}} > 1.$$

Let

$$a := \sqrt{4 + (\operatorname{Im} \zeta)^2} \geq 2,$$

$$b(a) := a - \frac{1}{a - 1 + \frac{1}{n-1}},$$

then we have

$$b(2) = 2 - \frac{1}{1 + \frac{1}{n-1}} = 2 - \frac{n-1}{n} = \frac{n+1}{n},$$

$$b'(a) = 1 + \frac{1}{\left(a - 1 + \frac{1}{n-1}\right)^2} > 1,$$

so that using the Taylor series for $b(a)$ at 2, we obtain

$$b(a) = b(2) + b'(2)(a-2) + \dots \geq \frac{n+1}{n} + (a-2) + \dots = a - \frac{n-1}{n} + \dots,$$

i.e. we obtain

$$\left| \tilde{F}_n(\zeta) \right| > b(a) \geq \sqrt{4 + (\operatorname{Im}\zeta)^2} - \frac{n-1}{n}.$$

□

Lemma 4.5.16. *If $|\operatorname{Re}\zeta| > 2$, then*

$$\operatorname{Re} \left(\tilde{F}_n(\zeta) \right) > 2 - \left(\sqrt{4 + (\operatorname{Im}\zeta)^2} - \frac{n-2}{n-1} \right)^{-1} > 1.$$

Proof. We have

$$\left| \operatorname{Re} \left(\tilde{F}_n(\zeta) \right) - \operatorname{Re}\zeta \right| < \frac{1}{\left| \tilde{F}_{n-1}(\zeta) \right|}$$

which implies using equation (4.78)

$$- \left(|\zeta| - \frac{1}{|\zeta| - 1 + \frac{1}{n-2}} \right)^{-1} < \operatorname{Re} \left(\tilde{F}_n(\zeta) \right) - \operatorname{Re}\zeta < \left(|\zeta| - \frac{1}{|\zeta| - 1 + \frac{1}{n-2}} \right)^{-1},$$

which then implies

$$\begin{aligned} \operatorname{Re} \left(\tilde{F}_n(\zeta) \right) &> \operatorname{Re}\zeta - \left(|\zeta| - \frac{1}{|\zeta| - 1 + \frac{1}{n-2}} \right)^{-1} \\ &> 2 - \left(|\zeta| - \frac{1}{|\zeta| - 1 + \frac{1}{n-2}} \right)^{-1} \\ &> 2 - \left(\sqrt{4 + (\operatorname{Im}\zeta)^2} - \frac{1}{\sqrt{4 + (\operatorname{Im}\zeta)^2} - 1 + \frac{1}{n-2}} \right)^{-1} > 1. \end{aligned}$$

Let

$$a := \sqrt{4 + (\operatorname{Im}(\zeta))^2},$$

$$d(a) := a - \frac{1}{a - 1 + \frac{1}{n-2}},$$

then we have

$$d(2) = 2 - \frac{1}{1 + \frac{1}{n-2}} = 2 - \frac{n-2}{n-1} = \frac{n}{n-1},$$

$$d'(a) = 1 + \frac{1}{\left(a - 1 + \frac{1}{n-2}\right)^2} > 1,$$

so that using the Taylor series expansion for $d(a)$ at 2

$$d(a) = d(2) + d'(2)(a-2) + \cdots \geq \frac{n}{n-1} + a - 2,$$

which implies

$$-(d(a))^{-1} \geq -\left(\frac{n}{n-1} + a - 2\right)^{-1} = -\left(a - \frac{n-2}{n-1}\right)^{-1},$$

i.e. we have

$$\operatorname{Re}\left(\tilde{F}_n(\zeta)\right) > 2 - \left(\sqrt{4 + (\operatorname{Im}\zeta)^2} - \frac{n-2}{n-1}\right)^{-1}.$$

□

4.5.3 Gershgorin-type localisation

4.5.3.1 Application of known results to the pencil problem

Recall that $\mathcal{A}_c = H_c^{(N)} + \lambda S$ is the linear pencil and $\mathbf{A}_c = S^{-1}H_c^{(N)}$ is the non-self-adjoint block matrix, and that $\operatorname{Spec}(\mathcal{A}_c) \equiv \operatorname{Spec}(\mathbf{A}_c)$. We already mentioned the Gershgorin set $\mathcal{G}(\mathbf{A}_c)$ of \mathbf{A}_c in Section 4.2.3. In this section, we apply the well-known Gershgorin-type eigenvalue localisations, mentioned in Section 2.2, to our problem. Note that, in this section, the letters i, j, p, q may represent different number sequences in each of the bullet points.

(i) The Brauer set $\mathcal{K}(\mathbf{A}_c)$ consists of seven different Brauer Cassini ovals given by

$$\begin{aligned} \mathcal{K}_{1,j}(\mathbf{A}_c) &= \mathcal{D}(c, \sqrt{2}), & \mathcal{K}_{i,j}(\mathbf{A}_c) &= \mathcal{D}(c, 2), \\ \mathcal{K}_{p,N}(\mathbf{A}_c) &= \mathcal{D}(-c, \sqrt{2}), & \mathcal{K}_{p,q}(\mathbf{A}_c) &= \mathcal{D}(-c, 2), \\ \mathcal{K}_{1,N}(\mathbf{A}_c) &= \{z \in \mathbb{C} : |z^2 - c^2| \leq 1\}, \\ \mathcal{K}_{i,N}(\mathbf{A}_c) &= \mathcal{K}_{1,q}(\mathcal{A}_c) = \{z \in \mathbb{C} : |z^2 - c^2| \leq 2\}, \\ \mathcal{K}_{p,j}(\mathcal{A}_c) &= \mathcal{K}_{i,q}(\mathcal{A}_c) = \{z \in \mathbb{C} : |z^2 - c^2| \leq 4\}, \end{aligned}$$

where $i, j = 2, \dots, n$ with $i \neq j$, and $p, q = n + 1, \dots, N - 1$ with $p \neq q$. Note that $\mathcal{K}_{1,j}(\mathbf{A}_c) \subset \mathcal{K}_{i,j}(\mathbf{A}_c)$, $\mathcal{K}_{p,N}(\mathbf{A}_c) \subset \mathcal{K}_{p,q}(\mathbf{A}_c)$, $\mathcal{K}_{1,N}(\mathbf{A}_c) \subset \mathcal{K}_{i,N}(\mathbf{A}_c) \subset \mathcal{K}_{p,j}(\mathbf{A}_c)$ and also $\mathcal{K}_{p,j}(\mathbf{A}_c) \subset \mathcal{K}_{i,j}(\mathbf{A}_c) \cup \mathcal{K}_{p,q}(\mathbf{A}_c)$. Then we obtain

$$\text{Spec}(\mathbf{A}_c) \subseteq \mathcal{K}(\mathbf{A}_c) = \mathcal{D}(c, 2) \cup \mathcal{D}(-c, 2),$$

which is the same region as the Gershgorin set.

(ii) We have from Theorem 2.2.5 that

$$\sum_{i=1}^N \frac{r_i(\mathbf{A}_c)}{\max_{j \in J_i} |a_{i,j}|} = 2 + 2(N - 2) = 2N - 2 \leq \alpha(1 + \alpha).$$

However, for any $n \geq 2$ (or $N \geq 4$), we have $\alpha \geq 2$, and so it gives a bigger region than Gershgorin set for our case.

(iv) The set $\Omega(\mathbf{A}_c)$ given in Theorem 2.2.6 produces a complicated expression and there is a freedom of choice of the set \tilde{J}_i . In addition, it takes a large amount of time to find the sets as n increases. Nevertheless, it gives a smaller region than the Gershgorin set for our case. First, we discuss this set in more detail at the end of this section. We then illustrate the set along with its comparison with other sets in Figure 4.7.

(v) Numerical experiments suggest that the set given in Theorem 2.2.7 gives the same region as the Gershgorin set when $c = 0$. However, the region gets much bigger as c increases. Therefore, we omit the mathematical argument for this set.

(vi) When we consider the sets given by Melman [51] and Li et al. [44], which were stated in Theorem 2.2.8 and Theorem 2.2.10 respectively, they both give the same region as the Gershgorin union.

(vii) Consider the union $\bigcup_{i=1}^N \mathcal{S}_i(H_c^{(N)}, S)$ given in Theorem 2.2.12. In our case, since $d_{i,j} = 0$ when $i \neq j$, the union yields the same region as the Gershgorin set.

(viii) The union $\bigcup_{i=1}^N \tilde{\mathcal{S}}_i(H_c^{(N)}, S)$ given in Theorem 2.2.13 consists of four different regions that are

$$\begin{aligned} \tilde{\mathcal{S}}_1(H_c^{(N)}, S) &= \left\{ z \in \mathbb{C} : \frac{|z - c|}{\sqrt{1 + |z|^2}} \leq 1 \right\}; \quad \tilde{\mathcal{S}}_j(H_c^{(N)}, S) = \left\{ z \in \mathbb{C} : \frac{|z - c|}{\sqrt{1 + |z|^2}} \leq 2 \right\}, \\ \tilde{\mathcal{S}}_k(H_c^{(N)}, S) &= \left\{ z \in \mathbb{C} : \frac{|z + c|}{\sqrt{1 + |z|^2}} \leq 1 \right\}; \quad \tilde{\mathcal{S}}_N(H_c^{(N)}, S) = \left\{ z \in \mathbb{C} : \frac{|z + c|}{\sqrt{1 + |z|^2}} \leq 2 \right\}, \end{aligned}$$

where $j = 2, \dots, n$ and $k = n + 1, \dots, N - 1$. Note that $\tilde{\mathcal{S}}_1(H_c^{(N)}, S) \subset \tilde{\mathcal{S}}_j(H_c^{(N)}, S)$ and $\tilde{\mathcal{S}}_N(H_c^{(N)}, S) \subset \tilde{\mathcal{S}}_k(H_c^{(N)}, S)$. Therefore we obtain

$$\text{Spec}(H_c^{(N)} - \lambda S) \subset \bigcup_{i=1}^N \tilde{\mathcal{S}}_i(H_c^{(N)}, S) \equiv \tilde{\mathcal{S}}_j(H_c^{(N)}, S) \cup \tilde{\mathcal{S}}_k(H_c^{(N)}, S),$$

which covers the whole complex plane when $|c| \leq 2$ and excludes a region when $|c| > 2$.

- (ix) Applying Gershgorin set for block matrices (b.m.) (Theorem 2.2.14) with $A_{11} = H_c$, $A_{22} = -H_c$ and $\|A_{12}\| = 1$ gives

$$\text{Spec}(\mathbf{A}_c) \subset \{\zeta \in \mathbb{C} : \text{dist}(\zeta, \text{Spec}(H_c) \cup \text{Spec}(-H_c)) \leq 1\},$$

which means that in the complex plane, there are n disks with centre $(\mu_j + c)$ and radius one; n disks with centre $(\mu_j - c)$ and radius one; and eigenvalues that lie within the union of $2n$ disks. In addition, we get

$$\text{Spec}(\mathbf{A}_c) \cap \mathbb{R} \subset [\mu_n - c, \mu_1 + c] \subset [-2 - c, 2 + c],$$

which was already known. Nevertheless, this result also supports that $\text{Im}\lambda \leq 1$ for all $n \in \mathbb{N}$.

- (x) Applying Brauer set for b.m. (Theorem 2.2.15) to our problem, we obtain

$$\text{Spec}(\mathbf{A}_c) \subset \{\zeta \in \mathbb{C} : \text{dist}(\zeta, \text{Spec}(H_c)) \text{dist}(\zeta, \text{Spec}(-H_c)) \leq 1\}.$$

As discussed above, some results do not give better bounds than Gershgorin Theorem when applied to the pencil \mathcal{A}_c problem. Namely, Fan and Hoffmann (Theorem 2.2.5) is worse for $n \geq 2$, Theorem 2.2.7 produces a bigger region when $c \neq 0$, and weighted Stewart-Sun (Theorem 2.2.13) gives nothing. On the other hand, some results do not improve classical Gershgorin, however they produce the same region as Gershgorin theorem. Namely, these are classical Brauer, Theorem 2.2.8 and Theorem 2.2.10, Unweighted Stewart-Sun (Theorem 2.2.12).

In addition to the ones which were mentioned in Section 2.2, there are many other Gershgorin-type regions which were obtained, for instance, by Ostrowski [79], Fan and Hoffman [79], Dashnic and Zusmanovich [18], Nakatsukasa [58], Li et al. [44], Anna et al. [17], Herzog and Schmoeger [29]. We, however, exclude these as they do not give a better spectral enclosure than the Gershgorin union for our particular case.

We note that we do not attempt to find the minimal Gershgorin set of \mathcal{A}_c as the algorithms are suitable for small or medium size matrices. This result was reviewed due to its importance.

In our case, there are three results which improve classical Gershgorin Theorem. Gershgorin set for b.m. given by Tretter in Theorem 2.2.14, Brauer set for b.m. given by Freingold-Varga in Theorem 2.2.15, and the set given by Melman in Theorem 2.2.6. We first turn our attention to the set $\Omega(\mathbf{A}_c)$ given by Melman in Theorem 2.2.6. We will compare these sets at the end of this subsection.

We choose $\tilde{J}_i \equiv J_i$ to obtain the smallest region. Let

$$\Omega(\mathbf{A}_c) = \tilde{\Omega}(\mathbf{A}_c) \cup \hat{\Omega}(\mathbf{A}_c)$$

where

$$\begin{aligned} \tilde{\Omega}(\mathbf{A}_c) &:= \bigcup_{i=1}^n \tilde{\Omega}_i(\mathbf{A}_c) = \bigcup_{i=1}^n \left\{ \bigcap_{j \in \tilde{J}_i} \Omega_{i,j}(\mathbf{A}_c) \right\}, \\ \hat{\Omega}(\mathbf{A}_c) &:= \bigcup_{k=n+1}^{2n} \hat{\Omega}_k(\mathbf{A}_c) = \bigcup_{k=n+1}^{2n} \left\{ \bigcap_{j \in \tilde{J}_k} \Omega_{k,j}(\mathbf{A}_c) \right\}. \end{aligned}$$

There are $2n$ sets in the union $\Omega(\mathbf{A}_c)$ and we divided the union into two; those whose centre are at c called $\tilde{\Omega}(\mathbf{A}_c)$ and those whose centre at $-c$ called $\hat{\Omega}(\mathbf{A}_c)$. In other words, $\tilde{\Omega}(\mathbf{A}_c)$ and $\hat{\Omega}(\mathbf{A}_c)$ are symmetric with respect to imaginary axis. Note that each set $\tilde{\Omega}_i(\mathbf{A}_c)$ consists of intersection of more than one regions, however we omit the mathematical expression of these sets for clarity and illustrate them instead. Numerical experiments suggest that when $n \geq 4$, the union $\tilde{\Omega}(\mathbf{A}_c)$ contains four possible geometric shapes and the union $\hat{\Omega}(\mathbf{A}_c)$ contains their symmetric regions with respect to the $\text{Im}\lambda$ -axis. We illustrate these regions in Figure 4.6, without specifying their centre. Nevertheless, when we take the union of these sets, we then see that

$$\bigcup_{i \in J_3} \tilde{\Omega}_i(\mathbf{A}_c) \subset \tilde{\Omega}_3(\mathbf{A}_c),$$

i.e. $\tilde{\Omega}(\mathbf{A}_c) \equiv \tilde{\Omega}_3(\mathbf{A}_c)$. Similarly, we have $\hat{\Omega}(\mathbf{A}_c) \equiv \hat{\Omega}_{2n-3}(\mathbf{A}_c)$.

Remark 4.5.17. The illustration of the set $\tilde{\Omega}_n(\mathbf{A}_c)$ in Figure 4.6 may change as c changes, however $\tilde{\Omega}_n(\mathbf{A}_c) \subset \tilde{\Omega}_3(\mathbf{A}_c)$ will always hold.

Looking at $\tilde{\Omega}_3(\mathbf{A}_c)$ and $\hat{\Omega}_{2n-3}(\mathbf{A}_c)$, we see that

$$\tilde{\Omega}_3(\mathbf{A}_c) = \bigcap_{j \in \tilde{J}_3} \Omega_{3,j}(\mathbf{A}_c) \equiv \{z \in \mathbb{C} : |z - c|^2 \leq 2|z - c| \text{ and } |z^2 - c^2| \leq 2|z + c|\}$$

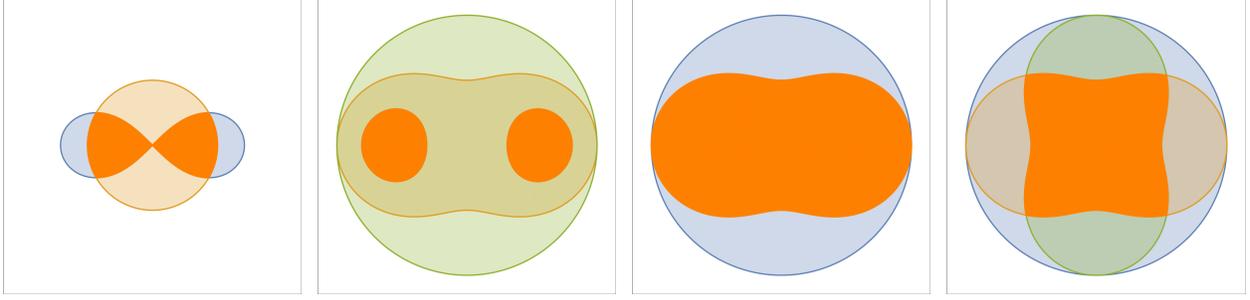


Figure 4.6: Without specifying their coordinates, four possible regions are illustrated from the union $\tilde{\Omega}(\mathbf{A}_c)$. Dark orange shaded regions from left to right: $\tilde{\Omega}_1(\mathbf{A}_c)$, $\tilde{\Omega}_2(\mathbf{A}_c)$, $\tilde{\Omega}_3(\mathbf{A}_c)$ and $\tilde{\Omega}_n(\mathbf{A}_c)$. Other coloured regions represent their corresponding intersected sets.

$$\begin{aligned} & \cap \{z \in \mathbb{C} : |(z - c)^2 - 1| \leq 1 + |z - c|\} \\ & \equiv \{z \in \mathbb{C} : |(z - c)^2 - 1| \leq 1 + |z - c|\}, \end{aligned}$$

and similarly

$$\hat{\Omega}_{2n-3}(\mathbf{A}_c) = \bigcap_{j \in \tilde{J}_{2n-3}} \Omega_{2n-3,j}(\mathbf{A}_c) \equiv \{z \in \mathbb{C} : |(z + c)^2 - 1| \leq 1 + |z + c|\}.$$

Hence

$$\text{Spec}(\mathbf{A}_c) \subset \Omega(\mathbf{A}_c) = \tilde{\Omega}_3(\mathbf{A}_c) \cup \hat{\Omega}_{2n-3}(\mathbf{A}_c).$$

We now compare these three sets in Figure 4.7. It seems that Gershgorin set for b.m. is contained in Brauer set for b.m., and they both support that $\text{Im}(\lambda) \leq 1$. On the one hand Tretter's result improves away on $\text{Re}(\lambda)$, on the other hand Freingold-Varga's result is better for small n , however it seems that the set is asymptotically the same as Gershgorin set for b.m. for large n . Moreover, the set $\Omega(\mathbf{A}_c)$ gives the same bound on $\text{Re}(\lambda)$ as classical Gershgorin and very close bound to the Gershgorin for b.m. on $\text{Im}(\lambda)$. However, when c is close to 2, it gives a better bound on $\text{Im}(\lambda)$ for the eigenvalues whose real parts are close to zero.

4.5.3.2 Gershgorin-type region for the two-parameter eigenvalue problem

Now, let us apply Corollary 2.2.16 to our problem. Let $A = H_0^{(n)}$, $D = H_0^{(m)}$ and $(C)_{n,1} = \kappa$, then we have

$$\text{Spec}_p(\mathbf{M}) \subset \mathcal{M} \left(H_0^{(n)}, H_0^{(m)} \right)$$

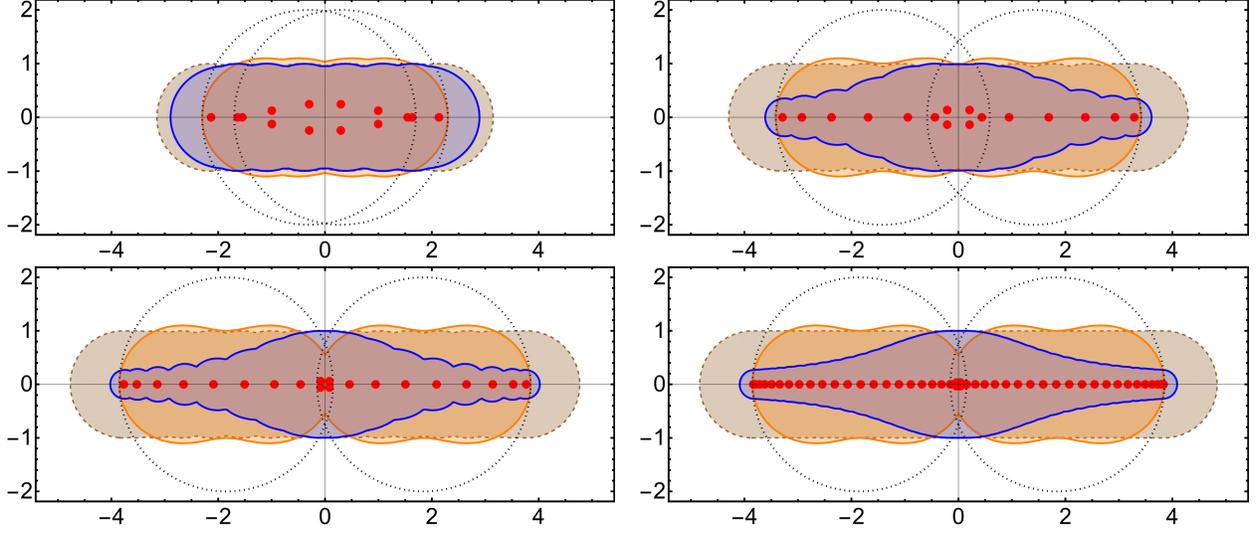


Figure 4.7: $\text{Spec}(\mathbf{A}_c)$ (red dots), the classical Gershgorin disks $\mathcal{G}(\mathbf{A}_c)$ (black dotted circles), Gershgorin sets for b.m. (brown shaded region), Brauer set for b.m. (blue shaded region) and Melman's set $\Omega(\mathbf{A}_c)$ (orange shaded region) are drawn for the non-self-adjoint matrix \mathbf{A}_c . Top-left: $c = 0.3$ and $n = 7$. Top-right: $c = \sqrt{2}$ and $n = 8$. Bottom-left: $c = 1.85$ and $n = 10$. Bottom-right: $c = 1.85$ and $n = 25$.

where

$$\mathcal{M}\left(H_0^{(n)}, H_0^{(m)}\right) = \left\{ (\alpha, \beta) \in \mathbb{C}^2 : \left(\inf_{a \in \text{Spec}(H_0^{(n)})} |\alpha - a| \right) \left(\inf_{d \in \text{Spec}(H_0^{(m)})} |\beta - d| \right) \leq \|C\|^2 \right\}$$

which can be re-written as

$$\mathcal{M}\left(H_0^{(n)}, H_0^{(m)}\right) = \bigcup_{i=1}^n \bigcup_{j=1}^m \left\{ (\alpha, \beta) \in \mathbb{C}^2 : \left| \alpha - \mu_i^{(n)} \right| \left| \beta - \mu_j^{(m)} \right| \leq \kappa^2 \right\},$$

where $\mu_i^{(n)} \in \text{Spec}\left(H_0^{(n)}\right)$. Illustration of Gershgorin-type localisation of the two-parameter eigenvalue problem in the $(\text{Re}(\alpha), \text{Re}(\beta))$ -plane can be seen for $n = m$ in Figure 4.8 and for $n \neq m$ in Figure 4.9.

4.5.3.3 Gershgorin circles under the mapping $z + 1/z$

In this section, we want to apply the Gershgorin Theorem to the problem (4.22) to obtain equivalent statements in terms of z and w values and we illustrate the region in the complex plane.

Let

$$\mu_j = 2 \cos \theta_j, \quad \theta_j = \pi j / (n + 1), \quad j = 1, \dots, n. \quad (4.82)$$

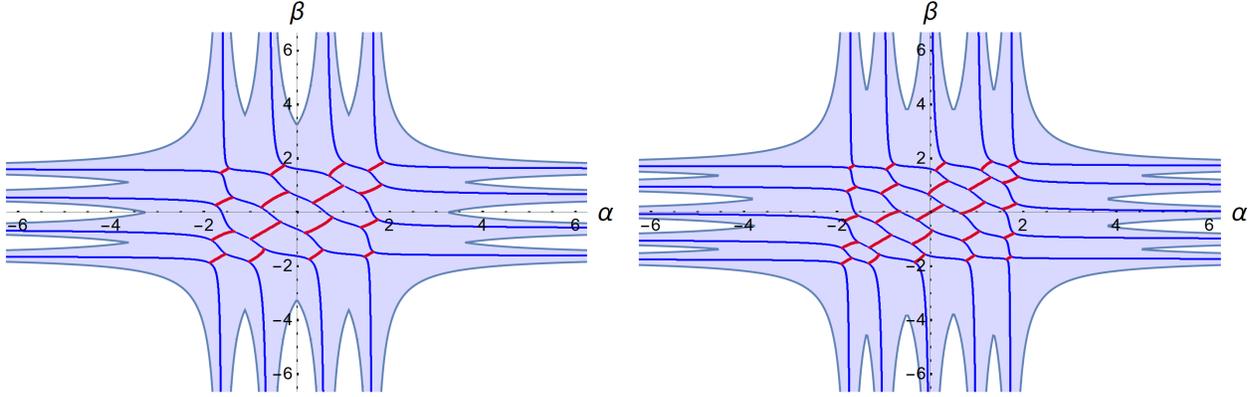


Figure 4.8: $\widetilde{\text{Spec}}(\mathbf{M})$ with $A = D = H_0^{(n)}$ and $\kappa = 1$, and blue shaded region is the union $\mathcal{M}(H_0^{(n)}, H_0^{(n)})$. Left: $n = 4$. Right: $n = 5$.

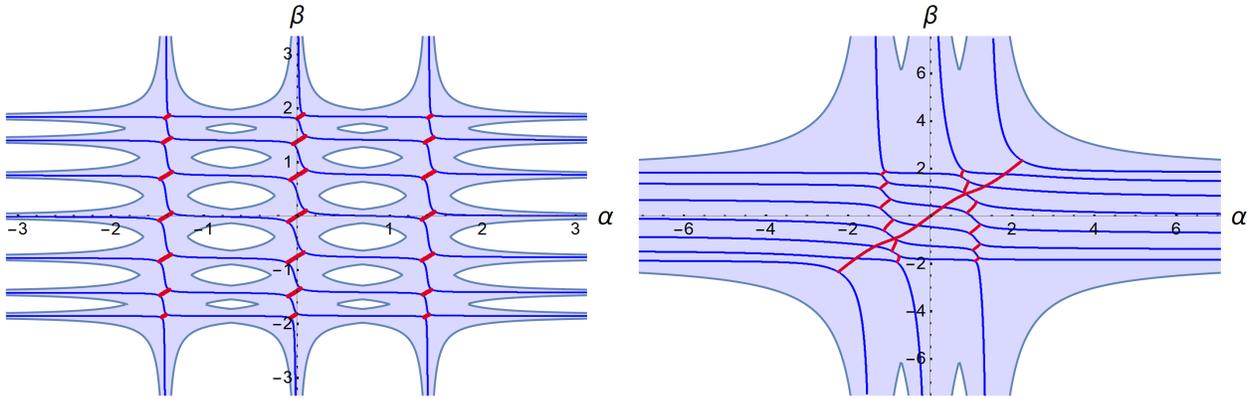


Figure 4.9: $\widetilde{\text{Spec}}(\mathbf{M})$ with $A = H_0^{(3)}$ and $D = H_0^{(7)}$ and blue shaded region is the union $\mathcal{M}(H_0^{(3)}, H_0^{(7)})$. Left: $\kappa = 0.3$. Right: $\kappa = \sqrt{3}$.

Recall that $\psi_{j,k} = \sqrt{\frac{2}{n+1}} \sin\left(\frac{\pi jk}{n+1}\right)$. Define

$$\widehat{r}_j := |\psi_{j,n}| \sum_{k=1}^n |\psi_{k,n}|. \quad (4.83)$$

Now, consider the problem (4.22):

$$\widetilde{\mathbf{A}}_c \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} \mu_1 + c & & & \psi_{1,n}\psi_{n,n} & \cdots & \psi_{1,n}\psi_{1,n} \\ & \ddots & & \vdots & & \vdots \\ & & \mu_n + c & \psi_{n,n}\psi_{n,n} & \cdots & \psi_{n,n}\psi_{1,n} \\ -\psi_{1,n}\psi_{n,n} & \cdots & -\psi_{1,n}\psi_{1,n} & -(\mu_1 + c) & & \\ \vdots & & \vdots & & \ddots & \\ -\psi_{n,n}\psi_{n,n} & \cdots & -\psi_{n,n}\psi_{1,n} & & & -(\mu_n + c) \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \\ v_1 \\ \vdots \\ v_n \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}.$$

Note that μ_j are symmetric. Then applying Gershgorin Theorem to $\tilde{\mathbf{A}}_c$ gives that

$$\text{Spec}(\tilde{\mathbf{A}}_c) \subset \mathcal{G}(\tilde{\mathbf{A}}_c) = \bigcup_{j=1}^n \mathcal{G}_j(\tilde{\mathbf{A}}_c),$$

where

$$\mathcal{G}_j(\tilde{\mathbf{A}}_c) = \mathcal{D}(\mu_j + c, \hat{r}_j) \cup \mathcal{D}(-\mu_j - c, \hat{r}_j).$$

To understand the geometry of $\mathcal{G}(\tilde{\mathbf{A}}_c)$, we illustrate each set in the union $\bigcup_j \mathcal{D}(\mu_j + c, \hat{r}_j)$ in Figure 4.10, without specifying its coordinates. Again, the union $\bigcup_j \mathcal{D}(\mu_j - c, \hat{r}_j)$ and $\bigcup_j \mathcal{D}(\mu_j + c, \hat{r}_j)$ are symmetric with respect to the imaginary axis. We then compare $\mathcal{G}(\tilde{\mathbf{A}}_c)$ and $\mathcal{G}(\mathbf{A}_c)$ in Figure 4.11.

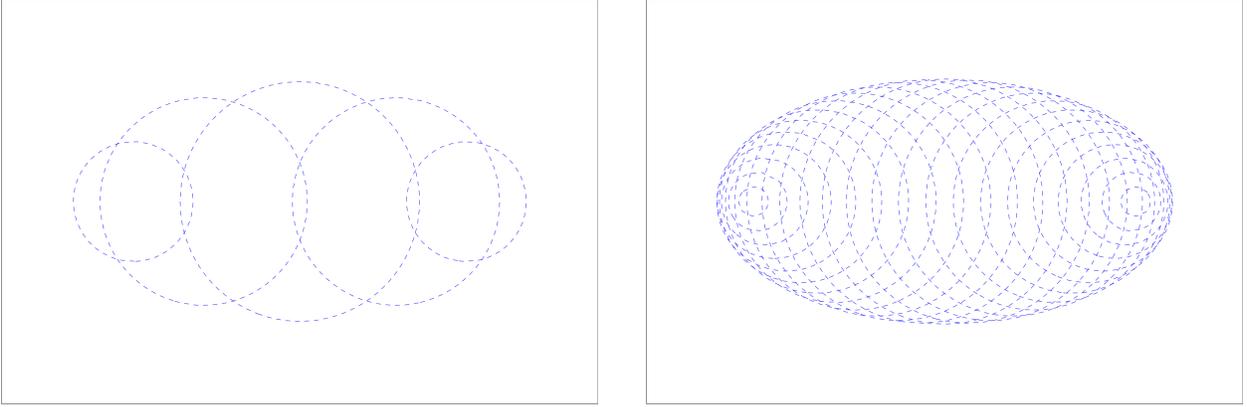


Figure 4.10: Without specifying the coordinates, each set in the union $\bigcup_j \mathcal{D}(\mu_j + c, \hat{r}_j)$ are drawn as blue dashed lines in $(\text{Re}(\lambda), \text{Im}(\lambda))$ -plane. Left: for $n = 5$. Right: for $n = 25$.

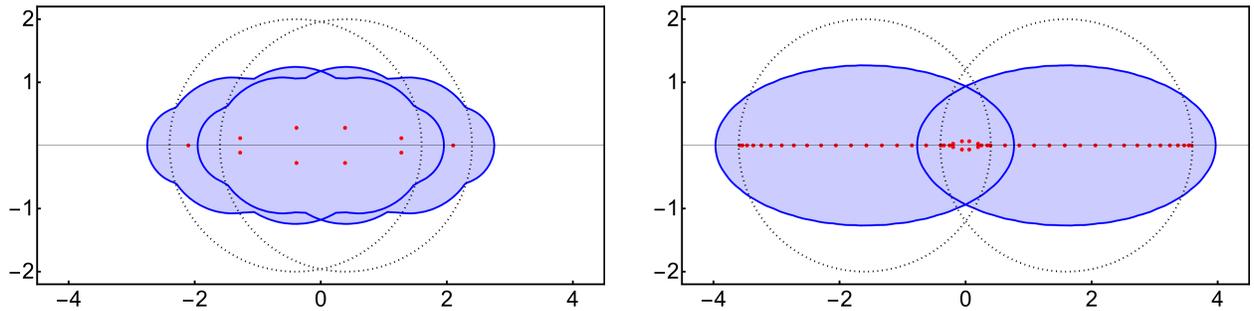


Figure 4.11: $\text{Spec}(\mathbf{A}_c)$ (red dots), the union $\mathcal{G}(\tilde{\mathbf{A}}_c)$ (blue shaded region) and the Gershgorin set $\mathcal{G}(\mathbf{A}_c)$ (black dotted circles) are drawn in $(\text{Re}\lambda, \text{Im}\lambda)$ -plane. Left: for $n = 5$ and $c = 0.4$. Right: for $n = 25$ and $c = 1.6$.

In order to plot the Gershgorin set $\mathcal{G}(\tilde{\mathbf{A}}_c)$ using the mapping $\lambda \mapsto z$ and $\lambda \mapsto w$ with (4.8), we need the following auxiliary result.

Lemma 4.5.18. *Let $\zeta \in \mathbb{C} \setminus \{0\}$, and μ_j and θ_j are as in (4.82). Then*

$$\left| \zeta + \frac{1}{\zeta} - \mu_j \right| = \frac{|\zeta - e^{i\theta_j}| |\zeta - e^{-i\theta_j}|}{|\zeta|}, \quad \left| \zeta + \frac{1}{\zeta} + \mu_j \right| = \frac{|\zeta + e^{i\theta_j}| |\zeta + e^{-i\theta_j}|}{|\zeta|}.$$

Proof. We prove the first of these equations, the second is similar. We have

$$\begin{aligned} \left| \zeta + \frac{1}{\zeta} - \mu_j \right| &= \frac{|\zeta^2 - \mu_j \zeta + 1|}{|\zeta|} \\ &= \frac{|\zeta^2 - 2\zeta \cos \theta_j + \cos^2 \theta_j + \sin^2 \theta_j|}{|\zeta|} \\ &= \frac{|(\zeta - \cos \theta_j)^2 - i^2 \sin^2 \theta_j|}{|\zeta|} \\ &= \frac{|\zeta - \cos \theta_j - i \sin \theta_j| |\zeta - \cos \theta_j + i \sin \theta_j|}{|\zeta|} \\ &= \frac{|\zeta - e^{i\theta_j}| |\zeta - e^{-i\theta_j}|}{|\zeta|}. \end{aligned}$$

□

Lemma 4.5.19. *Let λ, z, w be related by (4.8). Then λ is an eigenvalue of $\text{Spec}(\mathcal{A}_c)$ if and only if z and w lies in the union*

$$\mathcal{G}_\zeta := \bigcup_{j=1}^n \left\{ \zeta \in \mathbb{C} \setminus \{0\} : \frac{|\zeta - e^{i\theta_j}| |\zeta - e^{-i\theta_j}|}{|\zeta|} \leq \widehat{r}_j \right\}, \quad (4.84)$$

where θ_j and \widehat{r}_j are as in (4.82) and (4.83) respectively.

Proof. We have

$$|\lambda - \mu_j - c| = |\sigma - \mu_j| = \left| z + \frac{1}{z} - \mu_j \right|, \quad |\lambda + \mu_j + c| = |\tau + \mu_j| = \left| w + \frac{1}{w} + \mu_j \right|.$$

Applying Gershgorin Theorem to $\widetilde{\mathbf{A}}_c$ and then using Lemma 4.5.18 gives the union

$$\left\{ \zeta \in \mathbb{C} \setminus \{0\} : \frac{|\zeta - e^{i\theta_j}| |\zeta - e^{-i\theta_j}|}{|\zeta|} \leq \widehat{r}_j \right\} \cup \left\{ \zeta \in \mathbb{C} \setminus \{0\} : \frac{|\zeta + e^{i\theta_j}| |\zeta + e^{-i\theta_j}|}{|\zeta|} \leq \widehat{r}_j \right\}.$$

Note that there is a symmetry: $|\zeta - e^{i\theta_j}| = |\zeta + e^{i\theta_{n+1-j}}|$ and $|\psi_{j,k}| = |\psi_{n+1-j,k}|$. Therefore, when taking the union for all $j = 1, \dots, n$, the union reduces to \mathcal{G}_ζ due to the symmetries. We then have that $\lambda \in \text{Spec}(\mathcal{A}_c)$ iff $z, w \in \mathcal{G}_\zeta$ where \mathcal{G}_ζ is as given in (4.84). □

We illustrate each set in the union \mathcal{G}_ζ in Figure 4.12. Recall that if $\lambda \notin \mathbb{R}$, then $|z|, |w| > 1$. Note that the union consists of n sets and the boundary of each set is drawn with blue dashed lines. It can be seen that both the inner boundary and the outer boundary of the union \mathcal{G}_ζ get smoother as n increases. In Figure 4.13, we compare the region \mathcal{G}_ζ with the region $\mathcal{Z}_1 \cup \mathcal{Z}_2$, which was defined in Theorem 1.3.4(iv).

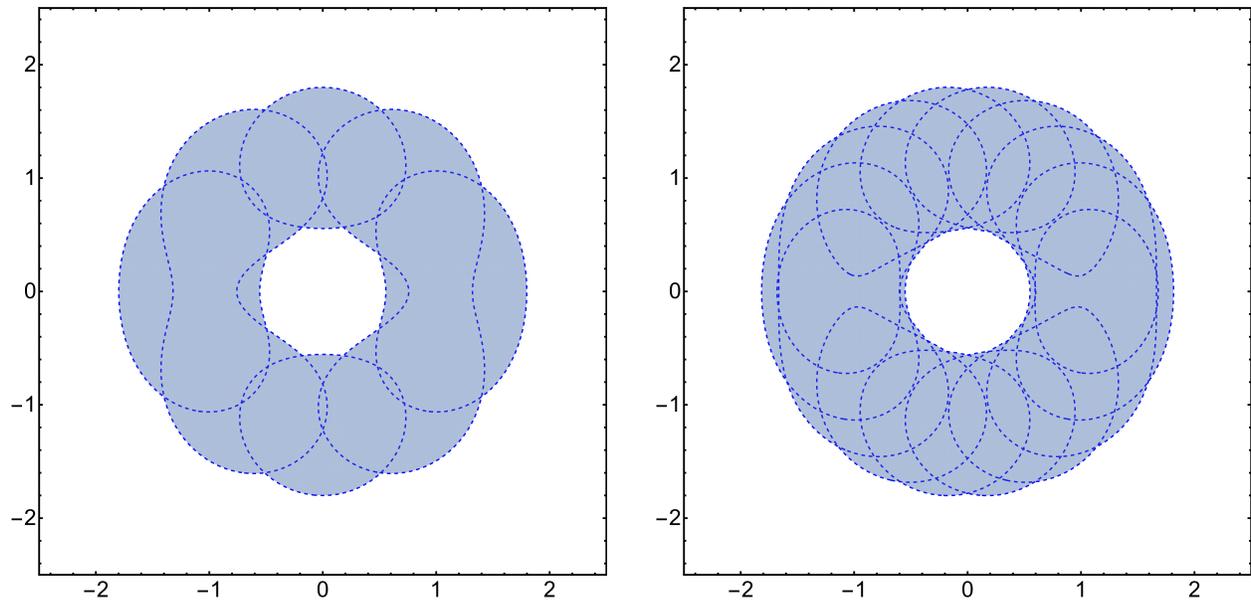


Figure 4.12: The union \mathcal{G}_ζ (blue shaded region) and the boundary of each set in the union \mathcal{G}_ζ (blue dashed lines) are drawn in the complex plane. Left: for $n = 5$. Right: for $n = 10$.

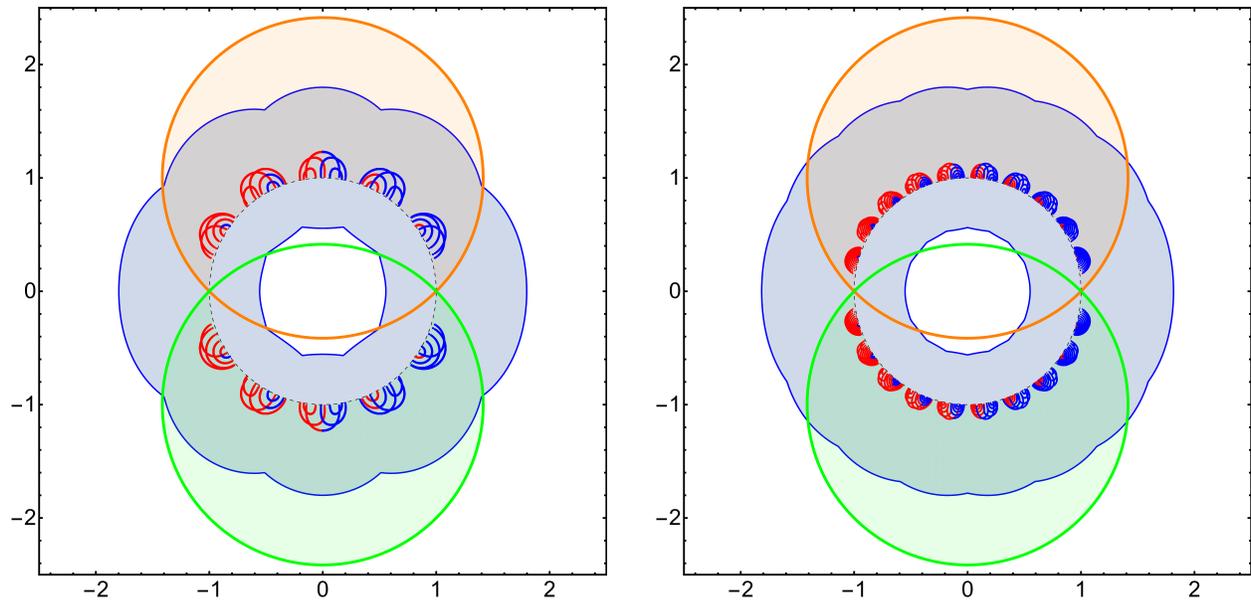


Figure 4.13: Superimposition of \mathcal{G}_ζ (blue shaded area), \mathcal{Z}_1 (orange shaded area), \mathcal{Z}_2 (green shaded area), z values (red dots) and w values (blue dots). Left: for $n = 5$. Right: for $n = 10$.

Chapter 5

Numerics and heuristics

In this chapter, we present some heuristics related to the non-real eigenvalues of a two-parameter eigenvalue problem and the pencil problem. There is a complicated interplay between the eigenvalues of the pencil \mathcal{A}_c . We start by describing the dynamics of the eigenvalues of \mathcal{A}_c as the parameter c changes in Section 5.1. In Section 5.2 we give illustrative examples related to a two-parameter eigenvalue problem. We examine the non-real pair-eigenvalues in different coordinate systems and we illustrate some interesting patterns in their location and behaviour. In Section 5.3, we conclude the chapter with a brief discussion of the double eigenvalues of \mathcal{A}_c . We propose several conjectures about the location and the quantity of double eigenvalues based on numerical experiments.

5.1 Dynamics of the eigenvalues of the pencil \mathcal{A}_c

When $c = 0$, all the eigenvalues of \mathcal{A}_c are non-real and Davies and Levitin [19] were able to determine the asymptotics of complex eigenvalues of \mathcal{A}_c as $n \rightarrow \infty$. However, as c changes, tracing the behaviour of the eigenvalues of \mathcal{A}_c remains difficult. In this section, we describe the dynamics of the eigenvalues of \mathcal{A}_c as c increases from 0 to 2. Since the spectrum $\text{Spec}(\mathcal{A}_c)$ is invariant under reflections about the real and imaginary axes, we are able to describe the behaviour that occurs in the right half plane, i.e. $\text{Re}(\lambda) > 0$. First, we recall the collision types from Figure 3.12; two real eigenvalues collide and produce a complex conjugate pair, called Type-A, and a complex conjugate pair collides and produces real eigenvalues, called Type-B.

Numerical experiments demonstrate that as c goes from 0 to 2, for arbitrary n each complex conjugate pair approach to each other along a curve, as opposed to a straight line, until they collide for the first time on the real axis. We refer to this as Level-1 which consists only of Type-B collisions that occur for the first time. All collisions in Level-1 occur

in order, i.e. the pair with the greatest real part collide first and the pair who has the least real part collide last.

After the first collisions occur, each pair travels along the real axis, where one heads to the right and the other to the left. If two real eigenvalues meet, they become a double eigenvalue at the point at which they meet. Subsequently they split and escape from the real line as a conjugate pair. In the complex plane, they make a small jump (in the sense that the eigenvalues travels a half-loop) in directions opposite to the origin. Then this jump is followed by another collision on the real line. This is what we refer to as Level-2, where eigenvalues have two collisions in total; first Type-A collisions occur and each complex conjugate pair makes a small jump in the complex plane and then Type-B collisions occur. The process in Level-2 is repeated in the following levels.

These collisions and jumps in each level are illustrated in Table 5.1 for $n = 7$. For simplicity, we plot jumps that occur only in the first quadrant. There are some collisions which takes place at the origin, i.e. $\lambda = 0$. When Type-A collisions occur at the origin, they then escape to the complex plane as a purely imaginary pair and they never leave the imaginary axis. They come back and collide on the real line at the origin again. Note that in Table 5.1 we do not show the jumps that occur at the origin in any level as the eigenvalues move along the imaginary axis only. However, the final collision always occurs at the origin.

We observe the following generic behaviour from numerics:

- (i) Each pair always collide, separately and independently of other pairs.
- (ii) All jumps occur in the direction opposite to the origin.
- (iii) At each Level- j , $j = 2, \dots, n - 1$, the eigenvalue whose real part is closest to the origin reaches higher point while jumping in the complex plane.
- (iv) At Level-1, the collisions are monotonic in c . This, however, is not true for any other levels. The collisions occur without order, that is for sufficiently large n , some eigenvalues at Level- j may be produced earlier than those which are still in Level- $(j - 1)$ or Level- $(j - 2)$. Nevertheless, collisions and jumps occur with sufficient speed such that the eigenvalues are unable to overtake each other on the real line.

5.2 Heuristics for the non-real pair-eigenvalues of M

In this section we discuss some heuristic results and conjectures for the behaviour of the non-real pair-eigenvalues of a two-parameter eigenvalue problem. The pair-eigenvalues

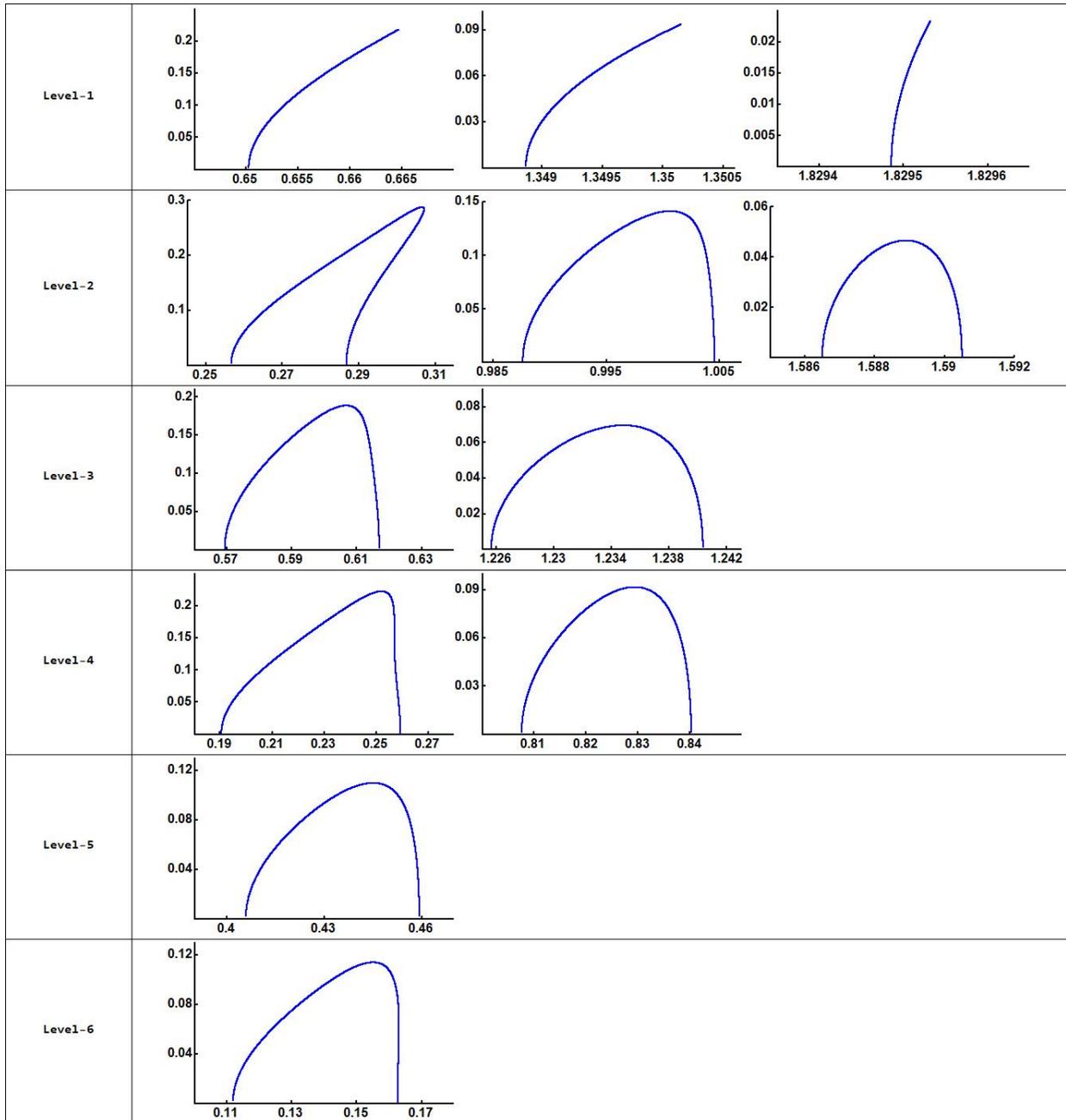


Table 5.1: For $n = 7$, blue dots represents the dynamics of the non-real eigenvalues of \mathcal{A}_c in the first quadrant of the complex plane $(\text{Re}(\lambda), \text{Im}(\lambda))$, as c increases from 0 to 2.

provide a better perspective in the $(c, \operatorname{Re}(\lambda))$ -plane than they do in the $(\operatorname{Re}(\alpha), \operatorname{Re}(\beta))$ -plane. We therefore present them in $(c, \operatorname{Re}(\lambda))$ coordinates. Recall the substitution (3.17),

$$\alpha - \beta = 2\lambda; \quad \alpha + \beta = -2c. \quad (5.1)$$

This substitution allows us to change the coordinate system from $(c, \operatorname{Re}(\lambda))$ to (α, β) . Therefore, we can equivalently write all results in Section 3.2 in the $(c, \operatorname{Re}(\lambda))$ -plane.

It appears from the numerical experiments that the patterns we show in here occur only for our specific example, that is, $\operatorname{Spec}_p(\mathbf{M})$ when $A = D = H_0$. Recall the two-parameter eigenvalue problem:

$$\begin{pmatrix} H_0 - \alpha & \kappa B \\ \kappa B & H_0 - \beta \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \mathbf{0}, \quad (5.2)$$

or equivalently

$$\mathbf{A}_{c,\kappa} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} H_c & \kappa B \\ -\kappa B & -H_c \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix},$$

where $\kappa \in \mathbb{R}$ and $B = B^*$ with $B_{n,n} = 1$ and all other entries of B are equal to zero. Note that when $\kappa = 1$, the problem is equivalent to the pencil problem considered in [19], i.e. $\mathbf{A}_c = \mathbf{A}_{c,1}$. In the following, we present some illustrations about the non-real-eigenvalues of $\mathbf{A}_{c,\kappa}$.

When $\kappa \geq 1$, the proportion of non-real eigenvalues of $\mathbf{A}_{c,\kappa}$ tends to usually decrease with κ , whereas $\kappa \leq 1$ it tends to increase with κ . We note that we show a typical picture for some $\kappa \geq 1$ in Figure 5.2(left). On the other hand, if we fix κ and change the size of the matrix n , then proportion of non-real eigenvalues becomes more stable, see Figure 5.2(right). Although the proportion of non-real eigenvalues become more stable for a specific value of c and κ as n increases, it remains difficult to estimate the range of possible values.

Another example is given in Figure 5.3 where we illustrate the eigenvalues which escape from the real line. In Figure 5.3, we take $n = 10$ and superimpose the real parts of the non-real eigenvalues of $\mathbf{A}_{c,\kappa}$, with respect to c , for different values of κ between 0.001 and 5. One can see a similar pattern to Chess Board structure in this figure, however, not in the real eigenvalues but in the non-real eigenvalues.

In the top panel of Figure 5.4, the non-real eigenvalues of $\mathbf{A}_{c,\kappa}$ is superimposed by taking n from 2 to 50. If one takes κ to be either closer to zero or large, then this pattern somehow gets clearer, see the bottom Figure 5.4 when $\kappa = 4$. In the next section, we will look at the escape points (i.e. collision points) in more details.

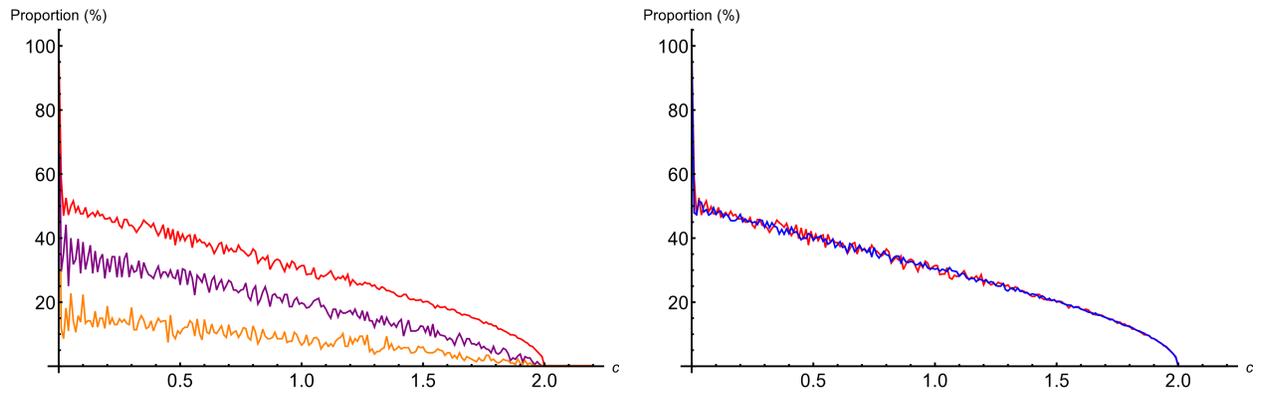


Figure 5.2: Proportion of the non-real eigenvalues of $A_{c,\kappa}$ as c goes from 0 to 2.2. Left: for $n = 500$, with $\kappa = 1$ (red line), $\kappa = 2$ (purple line), $\kappa = 5$ (orange line). Right: for $\kappa = 1$, with $n = 500$ (red line), $n = 1000$ (blue line).

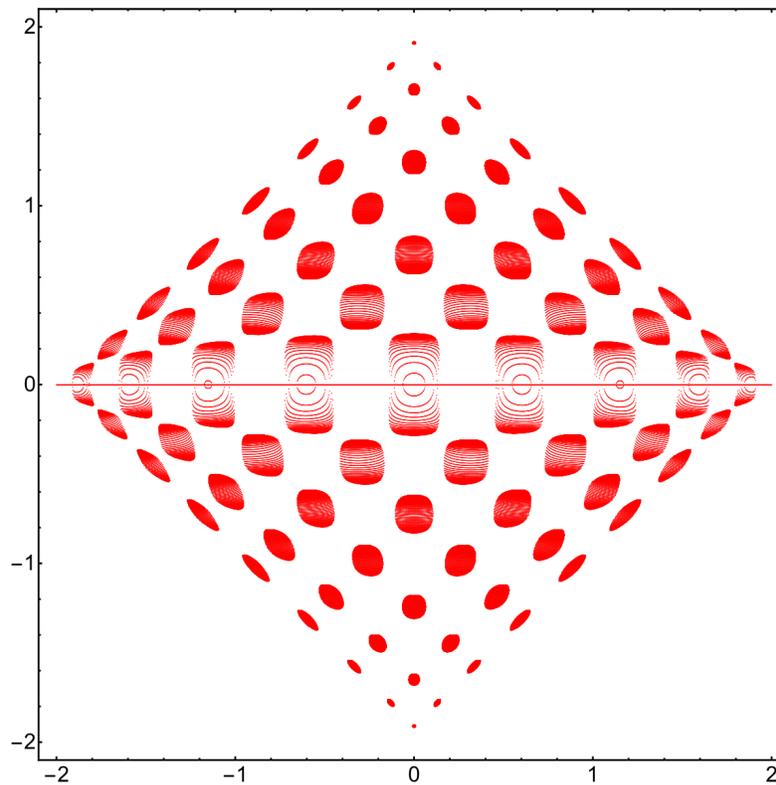


Figure 5.3: For $n = 10$, this figure shows the superimposition of the non-real eigenvalues of $A_{c,\kappa}$ in the $(c, \text{Re}(\lambda))$ -plane, when the values of κ ranges from 0.001 to 5 with the step-size of 0.04.

5.3 Double eigenvalues of \mathcal{A}_c

In this section we provide illustrative numerical examples for the location and the number of double eigenvalues of the pencil \mathcal{A}_c (or, equivalently $A_{c,1}$). Recall that the pencil \mathcal{A}_c has

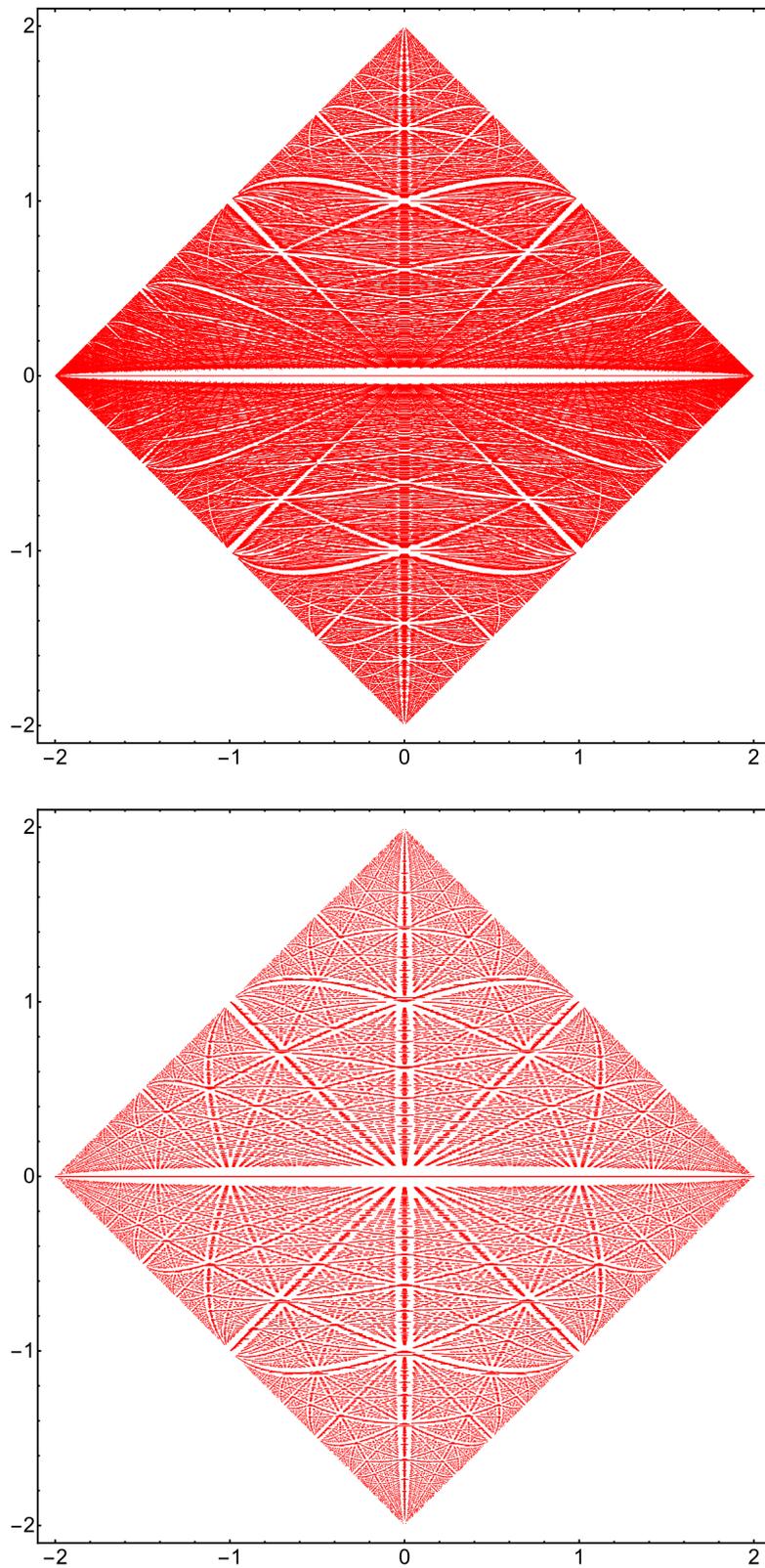


Figure 5.4: In the $(c, \text{Re}(\lambda))$ -plane, the superimposition of the non-real eigenvalues of $\mathbf{A}_{c, \kappa}$ by taking n from 2 to 50. Top: for $\kappa = 1$. Bottom: for $\kappa = 4$.

dimension $2n$. Most conjectures in this section are supported by numerical calculations for $n = 1, \dots, 30$ and for a wide range of c . As n gets bigger, it takes a relatively large amount of time to find the location of the double eigenvalues of \mathcal{A}_c . First, we note the following:

Conjecture 5.3.1. *For each given value of $n \in \mathbb{N}$ and $c \in (0, 2)$ there are no non-real double eigenvalues of \mathcal{A}_c .*

We provide two examples as illustrations. First, we plot all the double eigenvalues in the (c, λ) -plane for a fixed size, $n = 20$, in Figure 5.5. Although some double eigenvalues appear to lie on the same line, it is difficult to see a pattern. However, if one superimposes the double eigenvalues by taking the values of n from 2 to 30, then one would see that they form an interesting pattern in the (c, λ) -plane, as shown in Figure 5.6.

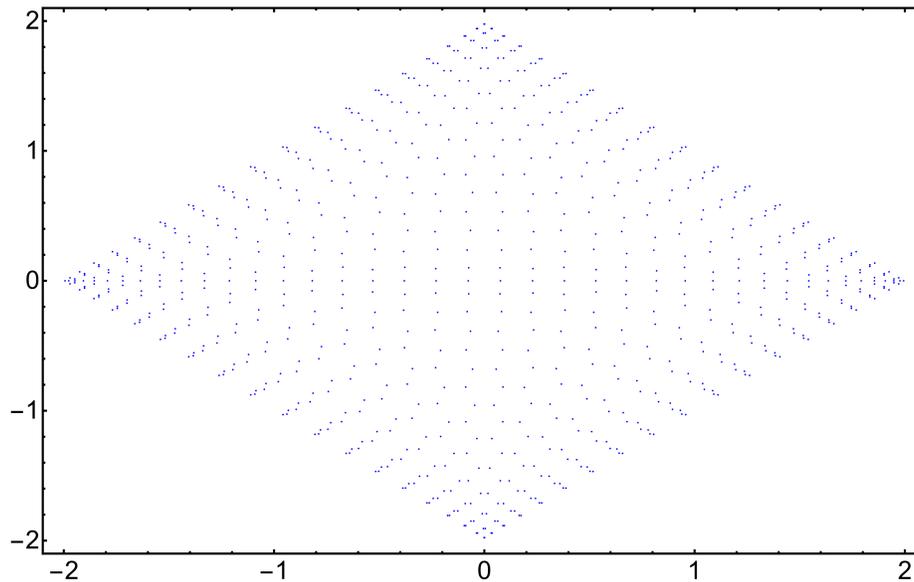


Figure 5.5: The double eigenvalues of \mathcal{A}_c in the (c, λ) -plane when $n = 20$.

As mentioned in Lemma 3.7.3, the collisions of the eigenvalues (or, equivalently, double eigenvalues) of the pencil \mathcal{A}_c occur when $dc/d\lambda = 0$ (or, equivalently $d\beta/d\alpha = -1$). These are the critical points along eigenvalue curves.

Assume that we are in the situation of the simple Chess Board Theorem. Recall from Chapter 3 that the real pair-eigenvalues of (5.2) when $\kappa = 1$ consists of curves $(\alpha, \beta(\alpha))$ which are continuous except at $\alpha \in \text{Spec}(H_0)$. We denote by Λ_i , $i = 1, \dots, n$, both branches of the curve $(\alpha, \beta_i(\alpha))$, such that $\beta_i(\alpha_i \pm 0) \rightarrow \pm\infty$. A typical enumeration of the curves Λ_i can be seen in Figure 5.7 for $n = 6$. Note that the eigenvalue curves

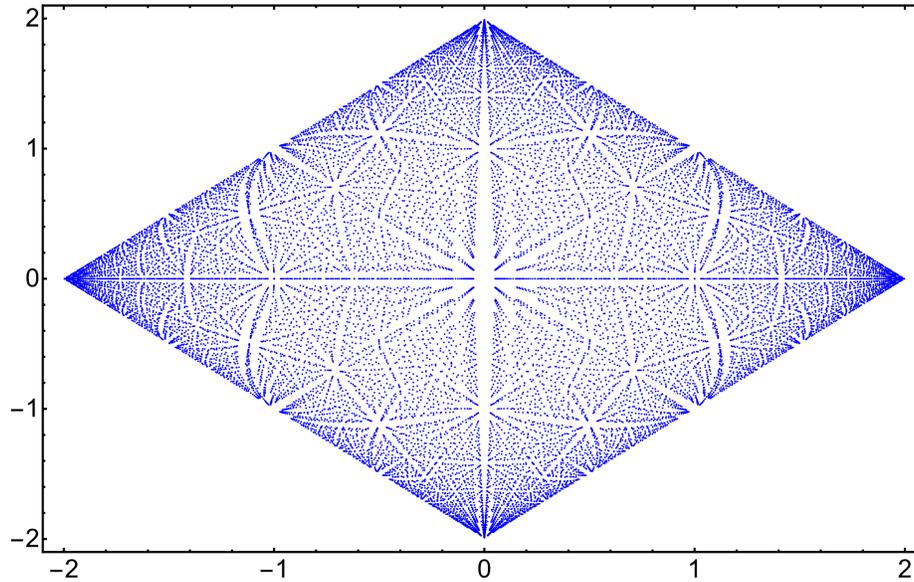


Figure 5.6: The superimposition of the double eigenvalues of \mathcal{A}_c in the (c, λ) -plane when n is between 2 and 30.

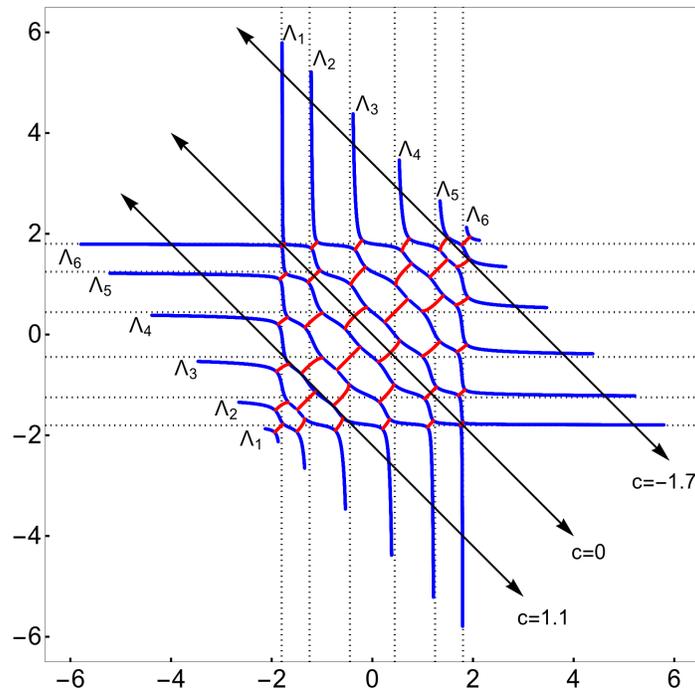


Figure 5.7: For $n = 6$, $\text{Spec}(\mathbf{A}_{c,1})$ when $c \in (-2, 2)$ in the $(\text{Re}(\alpha), \text{Re}(\beta))$ -plane. Black dotted lines represent $\alpha = \alpha_i \in \text{Spec}(H_0)$ in the vertical direction and $\beta = \alpha_i \in \text{Spec}(H_0)$ in the horizontal direction.

in Figure 3.11 look a bit different than they do in Figure 5.7. This is because we take $c \in (-2, 2)$ in Figure 5.7 whereas we considered $c \in \mathbb{R}$ in Figure 3.11.

From numerical experiments we observe the following:

Conjecture 5.3.2. *Let $c \in (-2, 2)$. Then each curve Λ_i , $i = 1, \dots, n$ has exactly $2n$ critical points such that*

$$\frac{d\beta_i(\alpha)}{d\alpha} = -1.$$

As can be seen from Figure 5.7 each curve has exactly n Type-A collisions and n Type-B collisions. We may be able to determine the location of some double eigenvalues of the pencil \mathcal{A}_c . Indeed, we can count the number of double eigenvalues of \mathcal{A}_c which occur at $\lambda = 0$. Recall the pencil problem

$$\mathcal{A}_c \mathbf{f} = (H_c^{(2n)} - \lambda S) \mathbf{f} = (H_0^{(2n)} + cI - \lambda S) \mathbf{f} = 0.$$

We observe that if $\lambda = 0$, then

$$H_0^{(2n)} \mathbf{f} = -c \mathbf{f},$$

which implies that $c = -\mu_j^{(2n)}$, and since $\mu_j^{(2n)}$ are symmetric, the double eigenvalues λ^* of \mathcal{A}_c that occur at the origin, i.e. at $\lambda = 0$, occur when

$$c = \mu_j^{(2n)} = 2 \cos \frac{\pi j}{2n+1}, \quad j = 1, \dots, 2n,$$

and therefore

$$\# \bigcup_{c \in (-2, 2)} \{\lambda^* \in \text{Spec}(\mathcal{A}_c) : \lambda^* = 0\} = 2n. \quad (5.3)$$

One should note that the real pair-eigenvalue spectrum viewed in $(\text{Re}(\alpha), \text{Re}(\beta))$ -plane covers the spectra of the corresponding pencils \mathcal{A}_c for all real c . To find the real eigenvalues of \mathcal{A}_{c_0} for a particular $c_0 \in \mathbb{R}$, one has to look at the intersection of the real eigenvalue curves (blue curves) with the straight line $\alpha + \beta = -2c$, see (5.1). Every line will intersect with the eigenvalue curves at most $2n$ points, cf. Figure 5.7. If, additionally, at each intersection point, the curve has gradient -1 , then it is a double eigenvalue intersection point. Note that for some particular c 's, there may be or may not be any double eigenvalues of \mathcal{A}_c since it is rare. So the number of all critical points as a union of all c 's and all λ 's is the number of double eigenvalues. Therefore λ^* do not depend continuously on c and they form a discrete set. If we look at the union of all c 's, then we look at the whole picture, c.f. Figure 5.5 for $n = 20$. On the other hand, in Figure 5.5, if one wants to look at the picture or count the double eigenvalues of \mathcal{A}_c for a given c , then one needs to take a straight vertical line in the (c, λ) -plane, and count how many of them are on the line, which will give the number of double eigenvalues.

Lemma 5.3.3. *Subject to Conjecture 5.3.2, for a fixed n , the double real eigenvalues λ^* of \mathcal{A}_c satisfy*

$$(i) \# \bigcup_{c \in (-2, 2)} \{\lambda^* \in \text{Spec}(\mathcal{A}_c) : -4 \leq \lambda^* \leq 4\} = 2n^2.$$

$$(ii) \# \bigcup_{c \in (-2, 2)} \{\lambda^* \in \text{Spec}(\mathcal{A}_c) : 0 < \lambda^*\} = n(n - 1).$$

Proof. The statement (i) follows by multiplying the number of curves, which is n , and the number of critical points in each curve, which is $2n$ by Conjecture 5.3.2. To prove (ii), using (5.3) we see that there are $2n^2 - 2n$ critical points which do not lie at $\lambda = 0$. Then the statement follows from dividing by 2, as we consider the upper-half plane $\lambda > 0$. \square

In the next result, we conjecture that all double eigenvalues of the pencil \mathcal{A}_c are localized to a specific area. Numerical experiments suggest that double eigenvalues of \mathcal{A}_c occur only when $\lambda < 2 - |c|$. In fact, if the only time when the eigenvalues of \mathcal{A}_c escape from the real line and rejoin the real line are after the collisions, then Conjecture 1.3.3 is a consequence of the following conjecture.

Conjecture 5.3.4. *The double eigenvalues λ^* of the pencil \mathcal{A}_c satisfy*

$$(i) \# \bigcup_{c \in (-2, 2)} \{\lambda^* \in \text{Spec}(\mathcal{A}_c) : 0 < \lambda^* + |c| < 2\} = n(n - 1),$$

$$(ii) \# \bigcup_{c \in (-2, 2)} \{\lambda^* \in \text{Spec}(\mathcal{A}_c) : 2 \leq \lambda^* + |c| \leq 4\} = 0.$$

Remark 5.3.5. Note that as c increases from 0 to 2, the double eigenvalues do not overtake each other when they collide and while they jump. Thus, Conjecture 5.3.4 implies that the rate at which eigenvalues become double eigenvalues should be lower than the rate at which c decreases.

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