STABILITY OF SOLUTIONS OF THE COMPLEX GINZBURG-LANDAU EQUATION

by

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To

Christine Johnson, my mother,

Joseph F. Gallo Jr., my late father,

and Noah Westerfield, a great friend gone too soon.

I couldn't have done it without you all.

STABILITY OF SOLUTIONS OF THE COMPLEX GINZBURG-LANDAU EQUATION

by

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STABILITY OF SOLUTIONS OF THE COMPLEX GINZBURG-LANDAU EQUATION

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Short-pulse lasers are modeled using equations related to the cubic-quintic complex Ginzburg-Landau equation (CQ-CGLE), which is a generalization of the nonlinear Schrödinger equation (NLSE). These lasers balance loss, gain, nonlinearity, spectral filtering, and dispersion in order to generate regular trains of stationary or periodically stationary pulses. While stationary pulses maintain a constant shape as they propagate, periodically stationary pulses change shape as they propagate around the laser loop, returning to the same shape once each round trip. With the advancement of laser technology, there has been a dramatic increase in the amount by which the pulses breathe each round trip of the laser. In this dissertation, we describe a method for determining the regions of parameter-space in which stable stationary pulses can be generated. Unlike other existing methods for finding stable stationary solutions, we anticipate that it will be possible to extend our proposed method to the case of periodically stationary pulses.

We describe the linearization of the the CQ-CGLE about a stationary solution, and we employ a method that uses the spectrum of the linearized operator to determine the stability of the pulse. The spectrum of the pulse is composed of the essential and point spectra, and while formulae exist for the essential spectrum, in general no such formulae exist for the point spectrum. We determine the point spectrum with the aid of a compact operator with a matrix-valued Green's kernel that is associated to the linearized operator.

We consider two types of compact operators, those which are trace class, and those which satisfy the weaker condition of being Hilbert-Schmidt. We review the theory of the Fredholm determinant of a trace class operator and the $2-$modified Fredholm determinant of a Hilbert-Schmidt operator, and we extend this theory to the case of matrix-valued kernels. We derive a formula for the numerical approximation of such Fredholm determinants and quantify the error between the true and approximated determinants. We then establish a result which quantifies when a Hilbert-Schmidt operator is trace class. We prove that if the matrix-valued Green's kernel associated to the linearization of the CQ-CGLE defines a trace class operator, then the Fredholm determinant of this operator is equal to the well-known Evans function.

Finally, we implement our numerical method in the special case of a known solution of the NLSE, and we show that in this case the kernel is trace class. We derive an explicit formula for the Evans function in this case and obtain excellent agreement between it and the numerically calculated Fredholm determinant. We quantify the behavior of the $2-$modified Fredholm determinant and present results showing the accuracy of our numerical method, thereby validating the error bounds we derived.

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INTRODUCTION

1.1 Lasers as Physical Motivation

The term laser refers to the acronym "Light Amplification by Stimulated Emission of Radiation." All lasers include some kind of gain medium, which amplifies light via stimulated emission. Fiber lasers, for instance, use optical fiber as the gain medium. Fiber lasers can be used in medicine, in material processing, in directed-energy weapons, and as sources of transmission in optical fiber communication systems. Fiber lasers generate regular trains of ultrashort pulses, the spectrum of which is referred to as a frequency comb. Applications of frequency combs include atomic clocks, precision-ranging laser radars, ultrasensitive chemical detectors, and high precision spectroscopy [1], [2], [3].

The behavior and stability of fiber laser systems is governed by the solutions of nonlinear wave equations that are related to the Nonlinear Schrödinger Equation (NLSE). Our goal is to prove theory about and develop a computational method for finding stable laser pulses which manifest themselves as solutions to these equations. Ultimately, we would like to show that this new approach is more widely applicable and computationally simpler than those already in common use.

The soliton laser is a short pulse mode-locked laser that generates soliton pulses in a single-mode fiber [4], [5]. By a soliton pulse, we mean one whose shape does not vary as the pulse propagates along the fiber. Since the development of the soliton laser, researchers have invented several other types of high-energy, short-pulse lasers. Dissipative soliton lasers, in which effects such as spectral filtering play a significant role, were introduced in about 2005 and are suitable for high energy applications [6], [7]. Similariton lasers were introduced in 2010 to create ultra-short pulses with a high tolerance to noise by exploiting the theoretical discovery of exponentially growing, self-similar pulses in optical fiber amplifiers [8], [9], [10],

[11], [12]. The most recent invention is the Mamyshev oscillator, which can produce pulses with a peak power in the Megawatt range. Each round trip of this laser, half of the pulse is destroyed before being regenerated again [13]-[14]. In summary, with the advancement of laser technology, there has been an increase in the amount by which pulses change shape over each round trip of the laser. Therefore, rather than creating soliton pulses which do not change over time, modern short-pulse lasers typically produce periodically stationary pulses, which change shape as they propagate but return to the same shape once per round trip of the laser. The basic reason the pulse changes shape as it propagates is that the laser loop consists of several components, each of which has a different effect on the pulse. These components are modeled using either nonlinear wave equations based on a nonlinear Schrödinger equation (NLSE) or discrete input-output transfer functions. The parameters in these models typically include dispersion, linear gain and loss, spectral filtering, nonlinear gain and loss, and a nonlinear refractive index. A key issue for experimentalists is to determine the regions of parameter-space in which stable pulses exist, and within that space, to optimize the pulse parameters for particular applications.

A lumped laser model is one in which models of the different components are concatenated together. Although lumped models are physically more realistic, they are harder to analyze mathematically. Instead, short-pulse lasers are often modeled using an averaged model, governed by a single constant-coefficient nonlinear wave equation in which the parameters represent average physical effects over one round trip of the laser. The most commonly used averaged model is based on the cubic-quintic complex Ginzburg-Landau equation (CQ-CGLE), which is a generalization of the NLSE. The CQ-CGLE admits both stationary and periodically stationary solutions, but in practice, the corresponding lasers generate periodic pulses of light, so we need a method which will be applicable to both types of solutions. While there are some analytical soliton solutions of the CQ-CGLE, there are no such analytical formulae for periodic solutions, except for the famous Kuznetsov-Ma (KM) breathers [15],

[16]. Nevertheless, there is significant numerical evidence for the existence of periodic pulses, such as those discovered by Akhmediev and his collaborators [17], [18].

In this dissertation, we explore a new numerical method for determining whether solutions of the CQ-CGLE are stable. This method involves the numerical calculation of Fredholm determinants of Birman-Schwinger operators. We will develop this method for stationary pulses. The major motivation for developing this new method is that it is highly unlikely that the Evans function methods described below can be extended to the case of periodically stationary pulses. However, we have reason to hope that our new method can be extended to the periodically stationary case. However, we leave this research project for future work.

1.2 Evans Function Method

The Evans function [19], [20], [21] is used to characterize the stability of stationary pulses in terms of a parameter, λ, in a first-order eigenvalue problem, such as in the case of the NLSE or the CQ-CGLE.

Given a stationary pulse solution of the NLSE or CQ-CGLE, we say that pulse is stable if, when we perturb the pulse slightly, the perturbation does not grow as it propagates through the system. In order to characterize this stability, we first linearize the nonlinear partial differential equation about a stationary pulse, Ψ, to obtain an associated linear differential operator, $\mathcal{L}(\Psi)$, and then ask whether there exist solutions of the linearized equation which grow. Equivalently, we ask if the eigenvalue equation $\mathcal{L}\mathbf{u} = \lambda\mathbf{u}$ has solutions λ for which $\text{Re}(\lambda) > 0$. If such solutions exist, we say the pulse Ψ is spectrally unstable. If, instead, $\text{Re}(\lambda) < 0$ for all λ in the spectrum of $\mathcal{L}$, then Ψ is a stable pulse. The spectrum, $\sigma(\mathcal{L})$, of $\mathcal{L}$ is composed of two parts, the essential spectrum, $\sigma_{\text{ess}}(\mathcal{L})$, and the point spectrum (or eigenvalues), $\sigma_{\text{pt}}(\mathcal{L})$. Formulae exist for the essential spectrum [22], but no such analytic solutions exist for the point spectrum, except in special cases. Therefore, in order to characterize the stability of a pulse Ψ, we must use a numerical method to compute $\sigma_{\text{pt}}(\mathcal{L})$.

Since we model the pulse Ψ as a function on the real line, we need to consider solutions $\mathbf{u}$ to the eigenvalue problem $(\mathcal{L} - \lambda)\mathbf{u} = 0$ which decay exponentially as the spatial variable $x \to \pm\infty$. This exponential decay guarantees that $\mathbf{u} \in L^2(\mathbb{R})$, so that $\lambda \in \sigma_{\rm pt}(\mathcal{L})$ holds. To define the Evans function, we fix a value $\lambda \in \mathbb{C}$ and consider two bases of solutions of the linearized operator called Jost solutions, those which satisfy appropriate $\lambda-$dependent exponential decay conditions as $x \to +\infty$, and those which satisfy similar decay conditions as $x \to -\infty$. If, at $x = 0$, the span of the Jost solutions from $x = -\infty$ has a nontrivial intersection with the span of the Jost solutions from $x = +\infty$, then these Jost solutions can be glued together to construct an eigenfunction $\mathbf{u} \in L^2(\mathbb{R})$. If this is the case, then the value of λ we fixed is an eigenvalue of $\mathcal{L}$, $\lambda \in \sigma_{\rm pt}(\mathcal{L})$ [20]. The Evans function, $E(\lambda)$, is a determinant constructed from the Jost solutions that is zero precisely when the spans of the Jost solutions have a nontrivial intersection at $x = 0$. That is, $E(\lambda) = 0$ if and only if $\lambda \in \sigma_{\rm pt}(\mathcal{L})$, with associated solution $\mathbf{u}$ that decays appropriately [20]. If all such eigenvalues λ are such that $\text{Re}(\lambda) < 0$, then the solution is said to be spectrally stable. It is assumed that this spectral stability will also imply linear stability, though such a result requires rigorous proof.

The Evans function method does, however, have its downfalls. Although the Evans function is useful for determining the stability of stationary solutions, it is not defined for periodically stationary solutions. In the case of a periodic solution, one could use Fourier series to derive an infinite-dimensional system of linearized equations for an analogue of the Jost solutions. However, finite-dimensional approximations of this system would be exceedingly stiff, which means that it is unlikely that such Jost solutions could be accurately computed, or even if they could be, that an Evans function could be theoretically defined for periodically stationary pulses. Instead, our aim is to develop a method which will work for characterizing stability of both solitons and periodically stationary pulses.

1.3 Birman-Schwinger Principle and Fredholm Determinants

Instead of using the Evans function method, we will use a method involving Birman-Schwinger operators and Fredholm determinants, as outlined in Chapters 2-4.

Similarly to the Evans function case, we linearize the differential equation about a solution Ψ and aim to compute the point spectrum of the linearized operator, $\mathcal{L}$. If the entirety of the point spectrum of $\mathcal{L}$ lies in the left half-plane, then the solution is considered stable. Rather than computing the roots of the Evans function, we compute the zeros of a Fredholm determinant associated with the linearized problem.

To utilize this method, we first introduce the Schatten $p-$classes, which are particular classes of compact operators defined on Hilbert spaces. In Chapter 2, we discuss trace class operators ($p = 1$) and the class of Hilbert-Schmidt operators ($p = 2$). We note that trace class operators are a strict subset of Hilbert-Schmidt operators. In Section 2.1, we review results from Teschl [23], Simon [24], Fredholm [25], and Bornemann [26] on the trace and Fredholm determinant of trace class operators on L^2-spaces on a compact interval that are defined in terms of scalar-valued kernels. Then, we generalize these results to the case of trace class operators on the real line that are defined in terms of matrix-valued kernels, which will be necessary to find stable solutions of the NLSE and CQ-CGLE. In Section 2.3, we discuss the case where an operator is Hilbert-Schmidt, but not necessarily trace class. We define the 2-modified Fredholm determinant of a Hilbert-Schmidt operator, and we review a formula for it in the case that the Hilbert-Schmidt operator is defined via a scalar-valued kernel on a compact interval [24]. Then, we generalize this result to derive a formula for the $2-$modified Fredholm determinant in the case of a matrix-valued kernel on the real line. This derivation relies on the von-Koch formula for block matrices and follows the proof style of Simon [24].

When determining the stability of a stationary solution, we classify the linearized operator, $\mathcal{L}$, for a fixed λ, based on its invertibility and Fredholm index. Using the well-known

Birman-Schwinger principle [27], [28], we construct a Hilbert-Schmidt integral operator, $\mathcal{K}(\lambda)$, on the real line, defined in terms of a Green's function for the linearized ordinary differential equation, which is given in terms of a matrix-valued kernel, $\mathbf{K}$. The operator $\mathcal{K}$ has the property that $\mathcal{K}(\lambda)$ is not invertible, i.e. that λ is in the point spectrum of $\mathcal{L}$, if and only if the 2−modified Fredholm determinant of $\mathcal{K}$ is equal to 0.

In the case of the NLSE or the CQ-CGLE, for instance, we must use a formula for Fredholm determinants of operators with matrix-valued kernels evaluated on the real line. Because the formula for these determinants involves an infinite sum of $n-$dimensional integrals over $\mathbb{R}^n$, it cannot be used in numerical computations. Instead, in Section 2.4, we approximate the Fredholm determinant by first truncating the integrals over $\mathbb{R}^n$ to integrals over $[-L, L]^n$, and then, in Section 2.5, we use a quadrature method to approximate these integrals. Our formulation for the quadrature error is obtained following a result from Bornemann [26] for operators on a finite interval. In addition, we derive a novel formula for the truncation error of this approximation. The error between the true Fredholm determinant and the approximation is less than the sum of the truncation and quadrature errors.

In this dissertation, we argue that this method is computationally simpler than the Evans function method. The Fredholm determinant, for fixed λ, is computed by simply forming a matrix and taking its determinant. Those values of λ which are roots of the Fredholm determinant can thereby be located using a simple root-finding method. This approach will enable us to determine the stability of a stationary pulse, and we anticipate this method can be adapted for periodic solutions as well [29].

1.4 A Result on Trace Class Kernels

Although there are several criteria which guarantee that a Hilbert-Schmidt operator is trace class [26, Section 2], none of them directly apply to Hilbert-Schmidt operators that are defined in terms of matrix-valued kernels on the real line. In Chapter 3, we prove a generalization of a classical result of Fredholm [25] which states, in essence, that a Hilbert-Schmidt operator with a Lipschitz-continuous kernel is trace class. Specifically, we extend Fredholm's theorem from the case of operators defined in terms of scalar-valued Hermitian-symmetric kernels on a compact interval to the more general case of matrix-valued kernels that are not assumed to have any symmetry properties. First, we establish this result for kernels on a compact interval, and then we extend it to the case of kernels on the real line. The proof relies on the work of Gohberg, Goldberg, and Krupnik [30] and Weidmann [31].

1.5 Fredholm Determinants and the CQ-CGLE

In Chapter 4, we apply the results from Chapters 2 and 3 to the case of the cubic-quintic complex Ginzburg-Landau equation (CQ-CGLE). Given a stationary solution $\Psi(x)$ of the CQ-CGLE, we define the associated second-order linear operator, $\mathcal{L}$, whose spectrum characterizes the linear stability of the stationary pulse. We additionally define the asymptotic operator, $\mathcal{L}_\infty$, which behaves like $\mathcal{L}$ does at spatial infinity. In Section 4.1, we define the first-order perturbed and unperturbed systems of equations, associated with the eigenvalue problems for $\mathcal{L}$ and $\mathcal{L}_\infty$, respectively, which are necessary to compute our Birman-Schwinger operator. We use the spectrum of the unperturbed system to help characterize the spectrum of the full, perturbed system.

In Section 4.2, we diagonalize the first-order unperturbed problem and calculate the eigenvalues and eigenvectors of the associated asymptotic matrix, $\mathbf{A}_\infty(\lambda)$. In Section 4.4, to define the integral operator $\mathcal{K}(\lambda)$ associated with the pulse Ψ, we apply the Birman-Schwinger principle. Then we discuss conditions on Ψ under which λ is in the point spectrum (is an eigenvalue) of $\mathcal{L}$. We discuss the decay conditions on the stationary pulse Ψ under which we can guarantee that our integral operator $\mathcal{K}$ is at least Hilbert-Schmidt. In Section 4.5, we define the matrix-valued integral kernel, $\mathbf{K}$, associated with our integral operator, and use our novel results from Chapter 2 to derive the formula for the 2−modified Fredholm determinant of $\mathcal{K}$ in terms of its kernel. We show that the eigenvalues of $\mathcal{L}$ are given by the zeros of the 2−modified Fredholm determinant of $\mathcal{K}$.

In Section 4.6, in order to apply our results from Chapter 3, we derive the conditions under which $\mathbf{K}$ is Lipschitz-continuous, and then we show that under these conditions, $\mathcal{K}$ is trace class. Consequently, the regular Fredholm determinant, $\det(\mathcal{I} + \mathcal{K}(\lambda))$, is defined, and the eigenvalues of $\mathcal{L}$ are then also given by the zeros of the regular Fredholm determinant of $\mathcal{K}$. In fact, we will see that the Fredholm determinant is equal to the Evans function [20]. This allows us to locate the point spectrum of $\mathcal{L}$ using the zeros of the Fredholm determinant, rather than the Evans function, while providing further evidence to support the validity of our method.

We must numerically approximate the Fredholm determinants for the CQ-CGLE, and in Section 4.8, we apply the error bounds we calculated in Sections 2.4 and 2.5 in this case.

1.6 Outline of Numerical Results

We recall that the NLSE is a special case of the CQ-CGLE, with some of the parameters set to zero. A well-known stationary solution of the NLSE, the sech solution, can be used in numerical simulations to test the accuracy of our method.

In Chapter 5, we study the Hilbert-Schmidt operator $\mathcal{K}$ associated with the sech solution of the NLSE. In particular, we explicitly calculate the matrix-valued kernel $\mathbf{K}(x, y)$ in this case, and we apply the results of Chapters 2, 3, and 4 to this kernel. We show that the hypotheses used in the theory apply to the sech solution, and that the integral operator $\mathcal{K}$ is, in fact, trace class. We explicitly calculate bounds on the error between the regular Fredholm determinant of $\mathcal{K}$ and its numerical approximation, as well as bounds on the error between the 2−modified Fredholm determinant and its numerical approximation. We observe convergence behaviors of the truncation and quadrature errors in this simulation and compare them to the our results from previous chapters.

Because $\lambda = 0$ is a known eigenvalue of the system, we observe the behaviors of the numerically approximated $\mathcal{K}(\lambda = 0)$ to determine a sufficiently large truncated interval and sufficiently small quadrature spacing so that we are able to calculate the matrix-valued kernel, $\mathbf{K}$, and the Fredholm determinants of $\mathcal{K}$, within a reasonable error. We expect that $\mathcal{K}(\lambda)$ and its Fredholm determinant will be most ill-behaved near the edge of the essential spectrum, which is explicitly computed for the sech solution of the NLSE.

In Section 5.2, we compute a formula for the Evans function associated with the sech solution of the NLSE following methods presented in [19] and [20]. Because we show that the Evans function is equivalent to the regular Fredholm determinant in the case of a trace class integral operator $\mathcal{K}$, we can compare the behavior of the Evans function $E(\lambda)$ to that of $\det(\mathcal{I} + \mathcal{K}(\lambda))$, for various values of λ. This bolsters our confidence in our approximation method, as the formula for $E(\lambda)$ is computed analytically.

In future work, the methods we have developed in this dissertation will be applied to analyze the stability of numerically-determined stationary pulse solutions of the CQ-CGLE.

CHAPTER 2

SCHATTEN-CLASS OPERATORS AND FREDHOLM DETERMINANTS

The Schatten $p-$classes are classes of compact operators on a Hilbert space. In this chapter, we discuss the two most important of these classes, the class of trace class operators ($p = 1$) and the class of Hilbert-Schmidt operators ($p = 2$). The class of trace class operators is a strict subset of the class of Hilbert-Schmidt operators. In Section 2.1, we review results from Teschl [23], Simon [24], Fredholm [25], and Bornemann [26] on the trace and Fredholm determinant of trace class operators, on L^2-spaces on a compact interval, that are defined in terms of scalar-valued kernels. Then, we generalize these results to the case of trace class operators on the real line that are defined in terms of matrix-valued kernels. In the case of matrix-valued kernels, the formula for the Fredholm determinant was first obtained by Fredholm in the special case of an operator on a compact interval. Our approach is based on a modern treatment of multilinear algebra on tensor and wedge product spaces, rather than on the ingeneous but somewhat ad-hoc methods of Fredholm.

In Section 2.2, we review the von-Koch formula for the Fredholm determinant of a block matrix $\mathbf{K}$. We extend this concept to derive a formula for the Fredholm determinant of a linear operator $\mathcal{K}$ evaluated on a finite interval. We will use this idea in Chapter 4 to derive our numerical approximation of $\det_p(\mathcal{I} + \mathcal{K})$, $p = 1$ or 2, for linear operator $\mathcal{K}$.

In Section 2.3, we discuss the case where the operator $\mathcal{K}$ is Hilbert-Schmidt, but not necessarily trace class. We define the 2-modified Fredholm determinant of a Hilbert-Schmidt operator, and we review a formula for it in the case that $\mathcal{K}$ defined via a scalar-valued kernel on a compact interval. Then, we generalize results from Simon [24] to derive a formula for the 2$-$modified Fredholm determinant in the case of a matrix-valued kernel on the real line.

Because the formula for these determinants involves an infinite sum over $n-$dimensional integrals, it cannot be used in numerical computations. Instead, in Section 2.4, we approximate the Fredholm determinant by first truncating the integrals over $\mathbb{R}^n$ to integrals over

$[-L, L]^n$, and then, in Section 2.5, we use a quadrature method to approximate these integrals. The error between the true Fredholm determinant and the approximation is less than the sum of the truncation and quadrature errors. We derive estimates for both of these errors. These results build upon a recent paper of Bornemann [26].

In Chapter 4, we will use the results in this chapter to study the stability of pulse solutions of the CQ-CGLE.

2.1 Trace Class Operators and the Fredholm Determinant

In this section, we review the definition of the trace and Fredholm determinant of a trace class operator on a Hilbert space. Our discussion follows that in Teschl [32] and Simon [24].

First, recall that a subset S of a normed space X is said to be *compact* if for every sequence of elements in S, there is a subsequence which converges to a point in S. A subset S of X is *relatively compact* if the closure of S is compact.

A linear operator $\mathcal{F} : X \to Y$ between normed spaces X and Y is said to be *compact* if $\mathcal{F}$ maps bounded sets in X to relatively compact sets in Y. We denote the set of compact operators from X to Y by $\mathcal{C}(X, Y)$, and let $\mathcal{C}(X) = \mathcal{C}(X, X)$.

We recall that a *Hilbert space,* $\mathcal{H}$, is a real or complex inner product space which is complete with respect to the norm induced by the inner product. Henceforth, we only consider Hilbert spaces that are separable. Let X and Y be real or complex Euclidean spaces, i.e. $\mathbb{R}^n$ or $\mathbb{C}^n$. The space $L^2(X, Y)$ is the Hilbert space of all square-integrable measurable functions from X to Y. We let $L^2(X) = L^2(X, X)$. For example, the set $L^2(\mathbb{R}, \mathbb{C}^n)$ is the space of square-integrable functions from $\mathbb{R}$ to $\mathbb{C}^n$ with the inner product

$$\langle \boldsymbol{\phi}, \boldsymbol{\psi} \rangle = \int_{\mathbb{R}} \boldsymbol{\phi}^*(x) \boldsymbol{\psi}(x) dx, \tag{2.1}$$

where $\boldsymbol{\psi}$ is $n \times 1$ and $\boldsymbol{\phi}^* = \overline{\boldsymbol{\phi}}^T$.

Let $\mathcal{F} : \mathcal{H} \to \mathcal{H}$ be a compact symmetric operator on an infinite dimensional Hilbert space. By the spectral theorem [32], there is a sequence of real eigenvalues $\lambda_j \to 0$ and an orthonormal set of eigenvectors ϕ_j of $\mathcal{F}$ so that for all $\psi \in \mathcal{H}$,

$$\mathcal{F}(\psi) = \sum_{j=1}^{\infty} \lambda_j \langle \phi_j, \psi \rangle \phi_j. \tag{2.2}$$

If $\mathcal{K} : \mathcal{H} \to \mathcal{H}$ is compact (but not necessarily symmetric), then $\mathcal{F} = \mathcal{K}^*\mathcal{K}$ is a compact symmetric operator, and so by (2.2), there are $\mu_j \in \mathbb{R}$ such that

$$\mathcal{K}^*\mathcal{K}(\psi) = \sum_{j=1}^{\infty} \mu_j^2 \langle \phi_j, \psi \rangle \phi_j. \tag{2.3}$$

A short calculation shows that $\mu_j = \|\mathcal{K}\phi_j\|$. The scalars μ_j are called the singular values of $\mathcal{K}$. Next, we recall a theorem from [32] on the singular value decomposition of compact operators.

Theorem 2.1.1 (Teschl pg. 89 [32])**.** *Let $\mathcal{K} \in \mathcal{C}(X, Y)$ be compact. Let μ_j be the singular values of $\mathcal{K}$ and $\{\phi_j\} \subset X$ the corresponding orthonormal eigenvectors of $\mathcal{K}^*\mathcal{K}$. Then*

$$\mathcal{K} = \sum_j \mu_j \langle \phi_j, \cdot \rangle \psi_j, \tag{2.4}$$

where $\psi_j = \mu_j^{-1}\mathcal{K}\phi_j$. The norm of $\mathcal{K}$ is given by the largest singular value

$$\|\mathcal{K}\| = \max_j \mu_j(\mathcal{K}). \tag{2.5}$$

Moreover, the vectors $\{\psi_j\} \subset Y$ are orthonormal and satisfy $\mathcal{K}^*\psi_j = \mu_j\phi_j$. In particular, ψ_j are the eigenvectors of $\mathcal{K}\mathcal{K}^*$ corresponding to the eigenvalues μ_j^2.

Definition 2.1.2 (Schatten $p-$classes)**.** *The* Schatten $p-$class *is the subspace of the space of all compact operators, $\mathcal{C}(\mathcal{H})$, defined by*

$$\mathcal{J}_p(\mathcal{H}) = \{\mathcal{K} \in \mathcal{C}(\mathcal{H}) : \|\mathcal{K}\|_p < \infty\}, \tag{2.6}$$

where

$$\|\mathcal{K}\|_p = \left(\sum_{j=1}^{\infty} |\mu_j|^p \right)^{1/p} = \|\mu\|_{\ell^p}, \tag{2.7}$$

with $\{\mu_j\}_{j=1}^{\infty}$ *being the singular values of* $\mathcal{K}$.

The two most important examples are the spaces $\mathcal{J}_1(\mathcal{H})$ of *trace class* operators, and the space $\mathcal{J}_2(\mathcal{H})$ of *Hilbert-Schmidt* operators. The following lemma shows that all trace class operators are also Hilbert-Schmidt.

Lemma 2.1.3. *For Hilbert space* $\mathcal{H}$,

$$\mathcal{J}_1(\mathcal{H}) \subseteq \mathcal{J}_2(\mathcal{H}). \tag{2.8}$$

Proof. Recall that $\ell^p = \{ \ \mathbf{a} = \{a_n\}_{n=1}^{\infty} : \sum_{n=1}^{\infty} |a_n|^p < \infty\}$ is a Banach space with norm

$$\|a_n\|_{\ell^p} = \left[\sum_{n=1}^{\infty} |a_n|^p \right]^{1/p}. \tag{2.9}$$

Let $\mathcal{K} \in \mathcal{J}_p(\mathcal{H})$ and let $\mu = \{\mu_n\}_{n=1}^{\infty}$ be the sequence of singular values of $\mathcal{K}$. Then by the definition of $\mathcal{J}_p(\mathcal{H})$,

$$\mathcal{K} \in \mathcal{J}_p(\mathcal{H}) \iff \mu \in \ell^p. \tag{2.10}$$

Since

$$\|\mu\|_{\ell^2} \leq \|\mu\|_{\ell^1}, \tag{2.11}$$

the result holds. □

It is well-known that the composition of a compact operator with a bounded operator is compact. A similar result holds for the Schatten p-classes [32, Theorem 3.1].

Proposition 2.1.4. *Let* $\mathcal{K} \in \mathcal{J}_p(\mathcal{H})$ *and let* $\mathcal{A} \in \mathcal{B}(\mathcal{H})$ *be a bounded operator. Then* $\mathcal{K} \circ \mathcal{A}$ *and* $\mathcal{A} \circ \mathcal{K}$ *are in* $\mathcal{J}_p(\mathcal{H})$.

Lemma 2.1.5 (Lemma 3.27, [32]). *If $\mathcal{K}$ is trace class, then the* trace $\mathrm{Tr} : \mathcal{J}_1(\mathcal{H}) \to \mathbb{C}$ *is the linear transformation defined by*

$$\mathrm{Tr}(\mathcal{K}) = \sum_k \langle \eta_k, \mathcal{K}\eta_k \rangle, \tag{2.12}$$

where $\{\eta_k\}$ is any orthonormal basis for $\mathcal{H}$. In particular,

$$|\,\mathrm{Tr}(\mathcal{K})| \leq \|\mathcal{K}\|_1, \tag{2.13}$$

is finite and independent of the choice of orthonormal basis.

Lidskii's theorem states that if $\mathcal{K}$ is a trace class operator with eigenvalues $\{\lambda_j\}$, counted according to algebraic multiplicity, then the trace is given by

$$\mathrm{Tr}(\mathcal{K}) = \sum_i \lambda_i(\mathcal{K}). \tag{2.14}$$

The following result gives yet another expression for the trace.

Theorem 2.1.6 (Theorem 3.1, [24]). *Let $\mathcal{K} \in \mathcal{J}_1(\mathcal{H})$ and suppose that, as in Theorem 2.1.1, that*

$$\mathcal{K} = \sum_{j=1}^{\infty} \mu_j(\mathcal{K}) \langle \phi_j, \cdot \rangle \psi_j. \tag{2.15}$$

Then

$$\mathrm{Tr}(\mathcal{K}) = \sum_{j=1}^{\infty} \mu_j(\mathcal{K}) \langle \phi_j, \psi_j \rangle. \tag{2.16}$$

Furthermore, if $\mathcal{A} \in \mathcal{B}(\mathcal{H})$ is bounded, then

$$\mathrm{Tr}(\mathcal{K}\mathcal{A}) = \mathrm{Tr}(\mathcal{A}\mathcal{K}). \tag{2.17}$$

Proof. Let $\mathcal{K} \in \mathcal{J}_1$ be defined as in (2.4), let $\{\eta_j\}$ be an orthonormal basis for $\mathcal{H}$, and let $a_{jk} = \langle \phi_j, \eta_k \rangle \langle \eta_k, \psi_j \rangle$. Then by Holder's inequality and Bessel's inequality,

$$\sum_k |a_{jk}| \leq \left(\sum_k |\langle \phi_j, \eta_k \rangle|^2 \right)^{1/2} \left(\sum_k |\langle \eta_k, \psi_j \rangle|^2 \right)^{1/2} \tag{2.18}$$

$$\leq \left(\|\phi_j\|^2 \right)^{1/2} \left(\|\psi_j\|^2 \right)^{1/2} \tag{2.19}$$

$$\leq 1. \tag{2.20}$$

Then by (2.15),

$$\sum_k |\langle \eta_k, \mathcal{K}\eta_k\rangle| \le \sum_{j,k} |a_{jk}|\mu_j(\mathcal{K}) \le \|\mathcal{K}\|_1, \tag{2.21}$$

which proves the inequality on $\mathrm{Tr}(\mathcal{K})$ found in Lemma 2.1.5. The absolute convergence of the double sum allows us to interchange the order of the summation to conclude that

$$\mathrm{Tr}(\mathcal{K}) = \sum_k \langle \eta_k, \mathcal{K}\eta_k\rangle = \sum_j \sum_k a_{jk}\mu_j(\mathcal{K}) = \sum_j \mu_j(\mathcal{K}) \sum_k a_{jk} = \sum_j \mu_j(\mathcal{K})\langle \phi_j, \psi_j\rangle. \tag{2.22}$$

The linearity of the trace follows from the absolute convergence of the sums. Finally, by (2.12) and (2.15), and by the orthonormality of the sets $\{\psi_j\}$ and $\{\phi_j\}$, we have that

$$\mathrm{Tr}(\mathcal{K}\mathcal{A}) = \sum_j \langle \psi_j, \mathcal{K}\mathcal{A}\psi_j\rangle = \sum_j \mu_j(\mathcal{K})\langle \phi_j, \mathcal{A}\psi_j\rangle = \sum_j \langle \phi_j, \mathcal{A}\mathcal{K}\phi_j\rangle = \mathrm{Tr}(\mathcal{A}\mathcal{K}). \tag{2.23}$$

□

The Fredholm determinant of a trace class operator $\mathcal{K}$ is defined in terms of the traces of the induced operators, $\wedge^k(\mathcal{K})$, on the wedge product spaces, $\wedge^k\mathcal{H}$. We define the antisymmetric tensor products, $\wedge^k\mathcal{H}$, of a Hilbert space $\mathcal{H}$ as follows [24, Section 1.5].

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces with inner products $\langle\cdot,\cdot\rangle_{\mathcal{H}_j}$. The tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ is a Hilbert space, $\mathcal{P}$, together with a bilinear mapping $\phi : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathcal{P}$, such that

1. $\langle \phi(x_1, y_1), \phi(x_2, y_2)\rangle_{\mathcal{P}} = \langle x_1, x_2\rangle_{\mathcal{H}_1}\langle y_1, y_2\rangle_{\mathcal{H}_2}$,

2. the closure of the set of all finite linear combination of the vectors $\phi(x, y)$ is equal to $\mathcal{P}$, and

3. we write $\phi(x, y)$ as $x \otimes y$, and $\mathcal{P}$ as $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Once a two-fold tensor product space has been defined, the n-fold tensor product spaces can be defined inductively. The n-fold tensor product space $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ can be concretely realized as follows.

For Hilbert spaces, $\mathcal{H}_1, \dots \mathcal{H}_n$, let $\text{Hom}(\mathcal{H}_1, \dots, \mathcal{H}_n)$ denote the set of multilinear maps $\ell : \mathcal{H}_1 \times \cdots \times \mathcal{H}_n \to \mathbb{C}$. Then $\text{Hom}(\mathcal{H}_1, \dots, \mathcal{H}_n)$ is a vector space. Given $\phi_j \in \mathcal{H}_j$, we define an element $\phi_1 \otimes \cdots \otimes \phi_n \in \text{Hom}(\mathcal{H}_1, \dots, \mathcal{H}_n)$ by $(\phi_1 \otimes \cdots \otimes \phi_n)(\psi_1, \dots, \psi_n) = \prod_j^n \langle \phi_j, \psi_j \rangle_{\mathcal{H}_j}$. Let $\text{Hom}_f(\mathcal{H}_1, \dots, \mathcal{H}_n)$ denote the set of all *finite* linear combinations of the $\phi_1 \otimes \cdots \otimes \phi_n$. The inner product on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is characterized by

$$\langle \phi_1 \otimes \cdots \otimes \phi_n, \psi_1 \otimes \cdots \otimes \psi_n \rangle = \prod_{j=1}^{n} \langle \phi_j, \psi_j \rangle_{\mathcal{H}_j}. \tag{2.24}$$

Then $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is the closure of $\text{Hom}_f(\mathcal{H}_1, \dots, \mathcal{H}_n)$ in $\text{Hom}(\mathcal{H}_1, \dots, \mathcal{H}_n)$. Let $\bigotimes^n \mathcal{H} = \mathcal{H} \otimes \cdots \otimes \mathcal{H}$ be the n-fold tensor product of $\mathcal{H}$. Given $\psi_1, \dots, \psi_n \in \mathcal{H}$, we define

$$\psi_1 \wedge \cdots \wedge \psi_n = \frac{1}{\sqrt{n!}} \sum_{\pi \in \sigma_n} (-1)^\pi \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)}, \tag{2.25}$$

where σ_n is the set of permutations on $\{1, \dots, n\}$ and $(-1)^\pi$ is the sign of the permutation π. Let $\wedge^n \mathcal{H}$ be the closure in $\bigotimes^n \mathcal{H}$ of the set of all finite linear combinations of the form $\psi_1 \wedge \cdots \wedge \psi_n$, and let $\wedge^0 \mathcal{H} = \mathbb{C}$. A straight-forward calculation yields the following result.

Lemma 2.1.7. *If $\{\phi_j\}_{j=1}^\infty$ is an orthonormal basis of $\mathcal{H}$, then*

$$(\phi_1 \wedge \cdots \wedge \phi_n, \psi_1 \wedge \cdots \wedge \psi_n) = \det((\phi_j, \psi_i)_{1 \le i,j \le n}). \tag{2.26}$$

Consequently, $\{\phi_{j_1} \wedge \cdots \wedge \phi_{j_n}\}_{j_1, \dots, j_n = 1}^\infty$ is an orthonormal basis for $\wedge^n \mathcal{H}$.

If $\mathcal{K} : \mathcal{H} \to \mathcal{H}$ is a linear operator, then there exists an induced linear operator $\mathcal{K} \otimes \cdots \otimes \mathcal{K} : \bigotimes^n \mathcal{H} \to \bigotimes^n \mathcal{H}$ so that

$$(\mathcal{K} \otimes \cdots \otimes \mathcal{K})(\phi_1 \otimes \cdots \otimes \phi_n) = \mathcal{K}\phi_1 \otimes \cdots \otimes \mathcal{K}\phi_n. \tag{2.27}$$

Clearly, $\mathcal{K} \otimes \cdots \otimes \mathcal{K}$ maps $\wedge^n \mathcal{H}$ into $\wedge^n \mathcal{H}$. We denote this operator by

$$\wedge^n(\mathcal{K}) : \wedge^n \mathcal{H} \to \wedge^n \mathcal{H}. \tag{2.28}$$

Proposition 2.1.8. *Suppose that* $\dim \mathcal{H} = n < \infty$*, and let* $\mathcal{K} : \mathcal{H} \to \mathcal{H}$ *be a linear operator with eigenvalues* $\lambda_1, \ldots, \lambda_n$*. Then for any* $k \in \{1, \ldots, n\}$*,*

$$\dim \wedge^k \mathcal{H} = \binom{n}{k}, \tag{2.29}$$

and the eigenvalues of $\wedge^n \mathcal{K}$ *are of the form* $\lambda_{j_1} \ldots \lambda_{j_k}$*, where* $j_1 < j_2 < \cdots < j_k$*. Therefore,*

$$\operatorname{Tr}\big(\wedge^k(\mathcal{K})\big) = \sum_{j_1 < \cdots < j_k} \lambda_{j_1} \ldots \lambda_{j_k}. \tag{2.30}$$

In particular, via the isomorphism $\wedge^n \mathcal{H} \cong \mathbb{C}$*, we have that*

$$\wedge^n(\mathcal{K}) = \det(\mathcal{K}). \tag{2.31}$$

Furthermore,

$$\sum_{k=0}^{n} \operatorname{Tr}(\wedge^k(\mathcal{K})) = \prod_{j=1}^{n} (1 + \lambda_j) = \det(\mathcal{I} + \mathcal{K}). \tag{2.32}$$

Since the determinant is not even a linear functional, it is far from obvious how to extend it to linear operators, $\mathcal{K}$, on an infinite dimensional space. The importance of (2.32) is that the determinant of $\mathcal{I}+\mathcal{K}$ can be expressed in terms of the traces of the linear operators $\wedge^k \mathcal{K}$. In the case that $\mathcal{K}$ is a trace class operator on an infinite-dimensional Hilbert space $\mathcal{H}$, the following result of [24] shows that we can use the analogue of (2.32) to define $\det(\mathcal{I} + \mathcal{K})$.

Theorem 2.1.9 (Simon pg. 33, [24])**.** *Suppose* $\mathcal{K}$ *is a trace class operator on separable Hilbert space* $\mathcal{H}$*. Then* $\wedge^k(\mathcal{K})$ *is a trace class operator on* $\wedge^k \mathcal{H}$ *and*

$$\big\|\wedge^k(\mathcal{K})\big\|_1 \le \frac{1}{k!} \|\mathcal{K}\|_1^k. \tag{2.33}$$

Consequently, the Fredholm determinant of $\mathcal{K}$*, defined by the series*

$$\det(\mathcal{I} + z\mathcal{K}) := \sum_{k=0}^{\infty} z^k \, Tr(\wedge^k(\mathcal{K})) \tag{2.34}$$

converges uniformly and absolutely to an entire function of z *such that*

$$|\det(\mathcal{I} + z\mathcal{K})| \le \exp(|z| \|\mathcal{K}\|_1). \tag{2.35}$$

2.2 The von-Koch Formula for Block Matrices

The famous von-Koch formula [26, Section 3] states that if $\mathbf{K} \in \mathbb{C}^{M\times M}$ is a matrix, and $z \in \mathbb{C}$, then

$$\det(\mathbf{I} + z\mathbf{K}) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{j_1,\ldots,j_n=1}^{M} \det\left([\mathbf{K}_{j_p,j_q}]_{p,q=1}^{n}\right) \tag{2.36}$$

can be expressed as a sum of determinants of submatrices of $\mathbf{K}$. This formula follows from the dependence of $\det(\mathcal{I} + z\mathcal{K})$ upon $\sum_n \mathrm{Tr}(\wedge^n \mathcal{K})$, which, when evaluated in terms of a Schur basis of $\mathcal{K}$, is built from the sum of all $n \times n$ principal minors of $\mathcal{K}$. This formula inspired Fredholm's definition of the Fredholm determinant of a trace class operator. Bornemann also used (2.36) in the derivation of a formula for a numerical approximation of the Fredholm determinant of a trace class operator on $L^2([a,b],\mathbb{C})$. We now derive a generalization of the von-Koch formula for block matrices that we will later use to obtain a numerical approximation of the Fredholm determinant of a trace class operator on $L^2(\mathbb{R},\mathbb{C}^k)$ that is defined in terms of a matrix-valued kernel.

Let $I_M = \{1, 2, 3, \ldots, M\}$, and let $L(I_M, \mathbb{C}^k)$ be the vector space consisting of all mappings $\phi : I_M \to \mathbb{C}^k$. Our goal is to derive a formula for $\det(\mathcal{I} + \mathcal{K})$, where $\mathcal{K}$ is a linear operator on $L(I_M, \mathbb{C}^k)$. Later, we will regard I_M as an index set for a discretization $\{x_1, \ldots, x_M\}$ of a finite interval I, in which case $L(I_M, \mathbb{C}^k)$ will discretize $L^2(I, \mathbb{C}^k)$.

First we observe that there is a vector space isomorphism

$$T : L(I_M, \mathbb{C}^k) \to \mathbb{C}^k \oplus \cdots \oplus \mathbb{C}^k \cong \mathbb{C}^{kM}, \tag{2.37}$$

given by

$$T(\phi) = (\phi(1), \ldots, \phi(M)). \tag{2.38}$$

We endow $L(I_M, \mathbb{C}^k)$ with the inner product

$$\langle \phi, \psi \rangle_{L(I_M,\mathbb{C}^k)} := \sum_{\ell=1}^{M} \langle \phi(\ell), \psi(\ell) \rangle_{\mathbb{C}^k}. \tag{2.39}$$

A basis for $L(I_M, \mathbb{C}^k)$ is given by

$$\mathcal{B} = \{\phi_{m,j} : m = 1, \ldots, M,\ j = 1, \ldots, k\}, \tag{2.40}$$

where

$$\phi_{m,j}(\ell) = \delta_{m\ell}\mathbf{e}_j, \tag{2.41}$$

and where $\mathbf{e}_j$ is the $j-$th standard basis vector in $\mathbb{C}^k$. The basis $\mathcal{B}$ is orthonormal, since

$$\begin{aligned}
\langle \phi_{m,i}, \phi_{n,j} \rangle &= \sum_{\ell=1}^{M} \langle \phi_{m,i}(\ell), \phi_{n,j}(\ell) \rangle_{\mathbb{C}^k} && (2.42)\\
&= \sum_{\ell=1}^{M} \langle \delta_{m\ell}\mathbf{e}_i, \delta_{n\ell}\mathbf{e}_j \rangle_{\mathbb{C}^k} && (2.43)\\
&= \delta_{mn} \langle \mathbf{e}_i, \mathbf{e}_j \rangle_{\mathbb{C}^k} && (2.44)\\
&= \delta_{nm}\delta_{ij}. && (2.45)
\end{aligned}$$

Therefore, for any $\phi \in L(I_M, \mathbb{C}^k)$, we have

$$\phi = \sum_{m,j} [\phi(m)]_j \phi_{m,j}. \tag{2.46}$$

Next, we let $\mathcal{K}$ be a linear operator on $L(I_M, \mathbb{C}^k)$. Then there exists $K_{m,i,n,j}$ such that

$$\mathcal{K}\phi_{m,i} = \sum_{n,j} K_{m,i,n,j}\phi_{n,j}. \tag{2.47}$$

We can arrange the tensor $K_{m,i,n,j}$ so that

$$K_{m,i,n,j} = [\mathbf{K}(n, m)]_{ji}, \tag{2.48}$$

where each $\mathbf{K}(n, m)$ is a $k \times k$ matrix with $(j, i)-$entry $K_{m,i,n,j}$. There are $M \times M$ such matrices $\mathbf{K}(n, m)$, and

$$\mathcal{K}\phi_{m,i} = \sum_{n=1}^{M} \sum_{j=1}^{k} [\mathbf{K}(n, m)]_{ji}\phi_{n,j}. \tag{2.49}$$

Claim: For any $\phi \in L(I_M, \mathbb{C}^k)$,

$$(\mathcal{K}\phi)(n) = \sum_{n=1}^{M} \mathbf{K}(n,m)\phi(m). \tag{2.50}$$

That is, the action of the operator $\mathcal{K}$ on ϕ is given in terms of a sum of matrix-vector products.

Proof. By (2.46), and by the linearity of $\mathcal{K}$,

$$\begin{aligned} \mathcal{K}\phi &= \sum_{m,i} [\phi(m)]_i \ \mathcal{K}\phi_{m,i} && (2.51) \\ &= \sum_{m,i,n,j} [\phi(m)]_i \ [\mathbf{K}(n,m)]_{ji}\phi_{n,j}, && (2.52) \end{aligned}$$

so that

$$\begin{aligned} (\mathcal{K}\phi)(\ell) &= \sum_{m,i,n,j} [\phi(m)]_i \ [\mathbf{K}(n,m)]_{ji}\phi_{n,j}(\ell) && (2.53) \\ &= \sum_{m,i,n,j} [\mathbf{K}(n,m)]_{ji} \ [\phi(m)]_i \delta_{n\ell}\mathbf{e}_j && (2.54) \\ &= \sum_m \sum_j [\mathbf{K}(\ell,m)\phi(m)]_j \mathbf{e}_j && (2.55) \\ &= \sum_m \mathbf{K}(\ell,m)\phi(m). && (2.56) \end{aligned}$$

□

Using the isomorphism (2.37), if we let

$$\mathbf{\Phi} = \begin{bmatrix} \phi(1) \\ \vdots \\ \phi(M) \end{bmatrix} = T(\phi) \in \mathbb{C}^{kM}, \tag{2.57}$$

then the action of $\mathcal{K}$ on ϕ is given by the block matrix multiplication

$$\mathcal{K}\phi = T^{-1}(\mathbf{K}(T(\phi))) \tag{2.58}$$

where $\mathbf{K}$ is the block matrix

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}(1,1) & \dots & \mathbf{K}(1,M) \\ \vdots & & \vdots \\ \mathbf{K}(M,1) & \dots & \mathbf{K}(M,M) \end{bmatrix} \in \mathbb{C}^{kM\times kM}. \tag{2.59}$$

With these preliminaries, we can generalize the von-Koch formula to block matrices, that is, to linear operators on $L(I_M, \mathbb{C}^k)$. We note that Fredholm already knew the formula in Theorem 2.2.1 in 1903 [25], using it in his study of systems of integral equations. However, the proof we provide here is more in line with the more recent approaches to Fredholm determinants, such as can be found in Simon [24].

Theorem 2.2.1. *Let $\mathcal{K}$ be a linear operator on $L(I_M, \mathbb{C}^k)$. Let*

$$\boldsymbol{\Phi}_{\boldsymbol{m},\boldsymbol{j}} = \phi_{m_1,j_1} \wedge \cdots \wedge \phi_{m_n,j_n} \in \wedge^n(L(I_M, \mathbb{C}^k)) \tag{2.60}$$

and let

$$\begin{aligned} \mathcal{M}_M^{(n)} &= \{\boldsymbol{m} = (m_1 \dots m_n) : 1 \le m_\alpha \le M \ \forall \alpha\}, & (2.61) \\ J_k^{(n)} &= \{\boldsymbol{j} = (j_1 \dots j_n) : 1 \le j_\alpha \le k \ \forall \alpha\}. & (2.62) \end{aligned}$$

Then

$$\mathrm{Tr}(\wedge^n \mathcal{K}) = \frac{1}{n!} \sum_{\boldsymbol{j}\in J_k^{(n)}} \sum_{\boldsymbol{m}\in\mathcal{M}_M^{(n)}} \langle \boldsymbol{\Phi}_{\boldsymbol{m},\boldsymbol{j}}, (\wedge^n\mathcal{K})\boldsymbol{\Phi}_{\boldsymbol{m},\boldsymbol{j}} \rangle_{\wedge^n(L(I_M,\mathbb{C}^k))}, \tag{2.63}$$

and consequently,

$$\det(\mathcal{I} + z\mathcal{K}) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{\boldsymbol{j}\in J_k^{(n)}} \sum_{\boldsymbol{m}\in\mathcal{M}_M^{(n)}} \det\left([\boldsymbol{K}(m_\alpha, m_\beta)]_{j_\alpha j_\beta} \right)_{\alpha,\beta=1}^n . \tag{2.64}$$

Remark. *To understand this definition of the Fredholm determinant in (2.64), we observe that $([\boldsymbol{K}(m_\alpha, m_\beta)]_{j_\alpha j_\beta})_{\alpha,\beta=1}^n$ is the $n \times n$ matrix whose $(\alpha,\beta)-$entry, $K_{j_\alpha j_\beta}(m_\alpha, m_\beta)$, is the $(j_\alpha, j_\beta)-$entry of the $k \times k$ matrix $\boldsymbol{K}(m_\alpha, m_\beta)$, which is one of the blocks of the $M \times M$ block matrix $\boldsymbol{K}$ in (2.59). Here, m_α, m_β are the α and β entries of the multi-index $\boldsymbol{m} =$*

$(m_1, \ldots, m_n) \in \mathcal{M}_M^{(n)}$. The formula for $\det(\mathcal{I} + z\mathcal{K})$ in (2.64) is given as an infinite sum over an index $n \in \mathbb{N}$ and multi-index $\boldsymbol{j} \in J_k^{(n)}$ of sums over $\mathcal{M}_M^{(n)}$. Because $\boldsymbol{K} \in \mathbb{C}^{kM \times kM}$, $\det(\mathcal{I} + z\mathcal{K})$ is a polynomial of degree kM in z. Therefore, the series in (2.64) must terminate at $n = kM$. Formula (2.64) for the Fredholm determinant of a matrix-valued operator on a finite interval is analogous to a formula we will derive for the Fredholm determinant of a trace class operator on the real line. We will use (2.64) in a derivation of a matrix determinant discretization of this Fredholm determinant.

Proof. Let

$$\mathcal{M}^{(n),\uparrow} = \{(\mathbf{m}, \mathbf{j}) \in \mathcal{M}_M^{(n)} \times J_k^{(n)} : (m_1, j_1) < \cdots < (m_n, j_n)\} \tag{2.65}$$

where $<$ denotes the lexicographic ordering defined such that $(m_1, j_1) < (m_2, j_2)$ if $m_1 < m_2$, or $m_1 = m_2$ and $j_1 < j_2$. Let

$$\mathcal{B}^{(n)} = \{\mathbf{\Phi}_{\mathbf{m},\mathbf{j}} : (\mathbf{m}, \mathbf{j}) \in \mathcal{M}^{(n),\uparrow}\}. \tag{2.66}$$

Then $\mathcal{B}^{(n)}$ is an orthonormal basis for $\wedge^n(L(I_M, \mathbb{C}^k))$. Let

$$\boldsymbol{\ell}^{(n)} = \{\boldsymbol{\ell} = (\mathbf{m}, \mathbf{j}) : 1 \leq m_\alpha \leq M,\ 1 \leq j_\alpha \leq k,\ \forall \alpha \in \{1, \ldots, n\}\}, \tag{2.67}$$

and let $\boldsymbol{\ell}^0$ be the set of indices in $\boldsymbol{\ell}^{(n)}$ with a repeated entry. Then

$$\boldsymbol{\ell}^{(n)} \setminus \boldsymbol{\ell}^0 = \{\pi(\boldsymbol{\ell}) = (\pi(\mathbf{m}), \pi(\mathbf{j})) : (\mathbf{m}, \mathbf{j}) \in \mathcal{M}^{(n),\uparrow}, \pi \in \sigma(n)\}, \tag{2.68}$$

and so

$$\begin{aligned} \sum_{\boldsymbol{\ell} \in \boldsymbol{\ell}^{(n)}} \langle \mathbf{\Phi}_{\boldsymbol{\ell}}, \wedge^n \mathcal{K} \mathbf{\Phi}_{\boldsymbol{\ell}} \rangle &= \sum_{\boldsymbol{\ell} \in \boldsymbol{\ell}^{(n)} \setminus \boldsymbol{\ell}^0} \langle \mathbf{\Phi}_{\boldsymbol{\ell}}, \wedge^n \mathcal{K} \mathbf{\Phi}_{\boldsymbol{\ell}} \rangle & (2.69) \\ &= \sum_{\boldsymbol{\ell} \in \mathcal{M}^{(n),\uparrow}} \sum_{\pi \in \sigma(n)} \langle \mathbf{\Phi}_{\pi(\boldsymbol{\ell})}, \wedge^n \mathcal{K} \mathbf{\Phi}_{\pi(\boldsymbol{\ell})} \rangle. & (2.70) \end{aligned}$$

Now, $\mathbf{\Phi}_{\pi(\boldsymbol{\ell})} = (-1)^\pi \mathbf{\Phi}_{\boldsymbol{\ell}}$, so by (2.25), (2.27), (2.68), and Lemma 2.1.5,

$$\begin{aligned} \sum_{\boldsymbol{\ell} \in \boldsymbol{\ell}^{(n)}} \langle \mathbf{\Phi}_{\boldsymbol{\ell}}, \wedge^n \mathcal{K} \mathbf{\Phi}_{\boldsymbol{\ell}} \rangle &= \sum_{\boldsymbol{\ell} \in \mathcal{M}^{(n),\uparrow}} \sum_{\pi \in \sigma(n)} \langle \mathbf{\Phi}_{\boldsymbol{\ell}}, \wedge^n \mathcal{K} \mathbf{\Phi}_{\boldsymbol{\ell}} \rangle & (2.71) \\ &= n! \sum_{\boldsymbol{\ell} \in \mathcal{M}^{(n),\uparrow}} \langle \mathbf{\Phi}_{\boldsymbol{\ell}}, \wedge^n \mathcal{K} \mathbf{\Phi}_{\boldsymbol{\ell}} \rangle & (2.72) \\ &= n! \operatorname{Tr}(\wedge^n \mathcal{K}). & (2.73) \end{aligned}$$

So,

$$\mathrm{Tr}(\wedge^n \mathcal{K}) = \frac{1}{n!} \sum_{\boldsymbol{\ell} \in \boldsymbol{\ell}^{(n)}} \langle \boldsymbol{\Phi}_{\boldsymbol{\ell}}, \wedge^n \mathcal{K} \boldsymbol{\Phi}_{\boldsymbol{\ell}} \rangle = \frac{1}{n!} \sum_{\mathbf{m} \in \mathcal{M}_M^{(n)}} \sum_{\mathbf{j} \in J_k^{(n)}} \langle \boldsymbol{\Phi}_{\mathbf{m},\mathbf{j}}, \wedge^n \mathcal{K} \boldsymbol{\Phi}_{\mathbf{m},\mathbf{j}} \rangle, \tag{2.74}$$

which proves (2.63).

Claim:

$$\langle \phi_{m,i}, \mathcal{K} \phi_{n,j} \rangle_{L(I_M, \mathbb{C}^k)} = [\mathbf{K}(m,n)]_{ij}. \tag{2.75}$$

Proof. By (2.50),

$$\begin{aligned} \langle \phi_{m,i}, \mathcal{K} \phi_{n,j} \rangle_{L(I_M, \mathbb{C}^k)} &= \sum_{\ell=1}^{M} \langle \phi_{m,i}(\ell), (\mathcal{K}\phi_{n,j})(\ell) \rangle_{\mathbb{C}^k} && (2.76) \\ &= \langle \mathbf{e}_i, \sum_{q=1}^{M} \mathbf{K}(m,q) \delta_{nq} \mathbf{e}_j \rangle_{\mathbb{C}^k} && (2.77) \\ &= \langle \mathbf{e}_i, \mathbf{K}(m,n) \mathbf{e}_j \rangle_{\mathbb{C}^k} && (2.78) \\ &= [\mathbf{K}(m,n)]_{ij}. && (2.79) \end{aligned}$$

□

Finally, substituting (2.74) into formula (2.32) for $\det(\mathcal{I} + \mathcal{K})$ and using

$$\langle \phi_1 \wedge \cdots \wedge \phi_n, \mathcal{K}\phi_1 \wedge \cdots \wedge \mathcal{K}\phi_n \rangle = \det\big[\langle \phi_i, \mathcal{K}\phi_j \rangle_{i,j=1}^{n} \big], \tag{2.80}$$

and (2.75), we obtain (2.64). □

2.3 Fredholm Determinants of Trace Class Integral Operators

In Section 2.1 we defined the trace and Fredholm determinant of a trace class operator on a general Hilbert space $\mathcal{H}$. Now, we consider an important special case, where $\mathcal{H}$ is an L^2-space. As noted in Lemma 2.1.3, all trace class operators are also Hilbert-Schmidt. As we recall, any Hilbert-Schmidt operator on an L^2-space is given by a kernel, $\mathbf{K}$. The question becomes how to calculate the trace and Fredholm determinant of $\mathcal{K}$ in terms of the kernel, $\mathbf{K}$.

Since the action of $\mathcal{K}$ on ϕ is given by an integral, which is analogous to matrix-vector multiplication, the formulae we will obtain are analogous to those for the trace and determinant of a matrix. Simon [24] and Fredholm [26] derived these formulae for scalar and matrix-valued kernels on a compact interval $[a, b]$. We extend these results to the case of matrix-valued kernels on $\mathbb{R}$, i.e. to operators on $L^2(\mathbb{R}, \mathbb{C}^k)$.

We first recall the following theorem from [24], which gives a criterion for ensuring that an operator on L^2 is Hilbert-Schmidt.

Theorem 2.3.1 (Simon pg. 23, [24])**.** *Let $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^n))$. Then, there exists a unique kernel $\boldsymbol{K} \in L^2(\mathbb{R} \times \mathbb{R}, \mathbb{C}^{n\times n})$ such that*

$$(\mathcal{K}\phi)(x) = \int_{\mathbb{R}} \boldsymbol{K}(x, y)\phi(y)dy, \tag{2.81}$$

and conversely, any kernel $\boldsymbol{K} \in L^2(\mathbb{R} \times \mathbb{R}, \mathbb{C}^{n\times n})$ defines an operator $\mathcal{K}$ which is in $\mathcal{J}_2$ and has $\|\mathcal{K}\|_2 = \|\boldsymbol{K}\|_2$, where $\|\mathcal{K}\|_2 = \int_{\mathbb{R}} \|\boldsymbol{K}\|^2_{\mathbb{C}^{n\times n}} < \infty$.

For our purposes, the most important part of this theorem is the converse statement, which states that if an operator is defined in terms of an L^2-kernel, then $\mathcal{K}$ is Hilbert-Schmidt. It is equally important to consider results which enable us to calculate the trace of integral operators that are trace class.

Theorem 2.3.2. *[Simon pg. 35, [24]] Let $\mathcal{K} \in \mathcal{J}_1(L^2([a, b], \mathbb{C}))$ be of the form*

$$(\mathcal{K}\phi)(x) = \int_a^b K(x, y)\phi(y)dy, \tag{2.82}$$

where K is continuous. Then

$$\operatorname{Tr}(\mathcal{K}) = \int_a^b K(x, x)dx. \tag{2.83}$$

Proof. Without loss of generality, let $[a, b] = [0, 1]$. Let $\mathcal{B}_n = \{\phi_{n,m}\}_{m=1}^{2^n}$ be the orthonormal set in $L^2([0, 1], \mathbb{C})$ given by

$$\phi_{n,m}(x) = \begin{cases} 2^{n/2}, & \frac{m-1}{2^n} < x < \frac{m}{2^n} \\ 0, & \text{otherwise.} \end{cases} \tag{2.84}$$

Let $\mathcal{P}_n$ be the projection onto $\mathrm{Span}(\mathcal{B}_n)$. We can construct an orthonormal basis $\{\psi_k\}_{k=1}^{\infty}$ for $L^2([0,1],\mathbb{C})$ so that $\psi_1,\ldots,\psi_{2^n} \in \mathrm{Ran}(\mathcal{P}_n)$. Then by Lemma 2.1.5,

$$\mathrm{Tr}(\mathcal{K}) = \lim_{n\to\infty} \mathrm{Tr}(\mathcal{P}_n\mathcal{K}\mathcal{P}_n), \tag{2.85}$$

where

$$\begin{aligned} \mathrm{Tr}(\mathcal{P}_n\mathcal{K}\mathcal{P}_n) &= \sum_{m=1}^{2^n} \langle \phi_{n,m}, \mathcal{K}\phi_{n,m}\rangle & (2.86)\\ &= 2^n \sum_{m=1}^{2^n} \iint\limits_{\chi_{n,m}} K(x,y)dxdy, & (2.87) \end{aligned}$$

where $\chi_{n,m} = \mathrm{Support}(\phi_{n,m}\otimes\phi_{n,m})$. On $\chi_{n,m}$,

$$K(x,y) \cong K\left(\frac{m}{2^n}, \frac{m}{2^n}\right), \tag{2.88}$$

and so

$$\begin{aligned} \mathrm{Tr}(\mathcal{P}_n\mathcal{K}\mathcal{P}_n) &\cong 2^n \sum_{m=1}^{2^n} \left(\frac{1}{2^n}\right)^2 K\left(\frac{m}{2^n}, \frac{m}{2^n}\right) & (2.89)\\ &= \sum_{m=1}^{2^n} \frac{1}{2^n} K\left(\frac{m}{2^n}, \frac{m}{2^n}\right) & (2.90)\\ &\cong \int_a^b K(x,x)dx. & (2.91) \end{aligned}$$

By the uniform continuity of K on the compact set $[0,1]\times[0,1]$, the error in (2.89) converges to 0 as $n\to\infty$. Similarly, by the continuity of $F(x) := K(x,x)$, and by the definition of a Riemann sum, the error in (2.91) also converges to 0 as $n\to\infty$. □

Next, we extend the previous theorem to the case of an integral operator $\mathcal{K}$ defined on all of $\mathbb{R}$ instead of on a finite interval $[a,b]$.

Theorem 2.3.3. *Let $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R},\mathbb{C}))$ be of the form*

$$(\mathcal{K}\phi)(x) = \int_{\mathbb{R}} K(x,y)\phi(y)dy, \tag{2.92}$$

where $K = K(x,y) \in L^2(\mathbb{R}\times\mathbb{R},\mathbb{C}) \cap C^0(\mathbb{R}\times\mathbb{R},\mathbb{C})$, *and suppose that* $F(x) := K(x,x) \in L^1(\mathbb{R},\mathbb{C})$. *Then*

$$\operatorname{Tr}(\mathcal{K}) = \int_{\mathbb{R}} K(x,x)dx. \tag{2.93}$$

Proof. Let $\mathcal{Q}_n : L^2(\mathbb{R},\mathbb{C}) \to L^2(\mathbb{R},\mathbb{C})$ be defined by

$$(\mathcal{Q}_n\phi)(x) = \chi_{[-n,n]}(x)\phi(x), \tag{2.94}$$

where $\chi_{[-n,n]}$ is the characteristic function of $[-n,n] \subset \mathbb{R}$. We can construct an orthonormal basis $\{\psi_m\}_{m=1}^{\infty}$ of $L^2(\mathbb{R},\mathbb{C})$ so that for every natural number n, there is a subsequence $\{\psi_{m_k^{(n)}}\}_{k=1}^{\infty}$, for which

$$\operatorname{Span}\{\psi_{m_k^{(n)}} : k = 1,2,\dots\} = \operatorname{Ran}(\mathcal{Q}_n) = L^2([-n,n],\mathbb{C}), \tag{2.95}$$

and

$$m^{(n)} := \left\{m_k^{(n)}\right\}_{k=1}^{\infty} \subseteq \left\{m_k^{(n+1)}\right\}_{k=1}^{\infty} \subseteq \cdots \subseteq \mathbb{N}, \tag{2.96}$$

with $\bigcup_{n=1}^{\infty} m^{(n)} = \mathbb{N}$. Now,

$$\operatorname{Tr}(\mathcal{Q}_n\mathcal{K}\mathcal{Q}_n) = \sum_{\ell\in m^{(n)}} \langle \psi_\ell, \mathcal{K}\psi_\ell\rangle, \tag{2.97}$$

as $\{\psi_\ell : \ell \in m^{(n)}\}$ is an orthonormal basis for $L^2([n,n])$. By Theorem 2.3.2, we have that

$$\operatorname{Tr}(\mathcal{Q}_n\mathcal{K}\mathcal{Q}_n) = \int_{[-n,n]} K(x,x)dx = \int_{\mathbb{R}} \chi_{[-n,n]}(x)K(x,x)dx. \tag{2.98}$$

Therefore,

$$|\operatorname{Tr}(\mathcal{K}) - \operatorname{Tr}(\mathcal{Q}_n\mathcal{K}\mathcal{Q}_n)| = \left|\sum_{\ell\notin m^{(n)}} \langle \psi_\ell, \mathcal{K}\psi_\ell\rangle\right| \leq \sum_{\ell\notin m^{(n)}} |\langle \psi_\ell, \mathcal{K}\psi_\ell\rangle|. \tag{2.99}$$

Let $\epsilon > 0$. Then, since $\mathcal{K}$ is trace class, $\exists M \in \mathbb{N}$ such that

$$\sum_{\ell > M} |\langle \psi_\ell, \mathcal{K}\psi_\ell\rangle| < \epsilon. \tag{2.100}$$

Since $\bigcup_{n=1}^{\infty} m^{(n)} = \mathbb{N}, \exists N$ such that $\{1, \ldots, M\} \subseteq m^{(N)}$. Then

$$\begin{aligned}
|\operatorname{Tr}(\mathcal{K}) - \operatorname{Tr}(\mathcal{Q}_N \mathcal{K} \mathcal{Q}_N)| &\leq \sum_{\ell \notin m^{(N)}} |\langle \psi_\ell, \mathcal{K}\psi_\ell \rangle| && (2.101)\\
&\leq \sum_{\ell > M} |\langle \psi_\ell, \mathcal{K}\psi_\ell \rangle| && (2.102)\\
&< \epsilon. && (2.103)
\end{aligned}$$

Therefore, by the definition of trace, and by Theorem 2.3.2,

$$\begin{aligned}
\operatorname{Tr}(\mathcal{K}) &= \lim_{n\to\infty} \operatorname{Tr}(\mathcal{Q}_n \mathcal{K} \mathcal{Q}_n) && (2.104)\\
&= \lim_{n\to\infty} \int_{\mathbb{R}} \chi_{[-n,n]}(x) K(x,x) dx && (2.105)\\
&= \int_{\mathbb{R}} K(x,x) dx. && (2.106)
\end{aligned}$$

To prove (2.106), we apply the Lebesgue Dominated Convergence Theorem, which holds since $|\chi_{[-n,n]} F| \leq |F|$, where $F \in L^1(\mathbb{R}, \mathbb{C})$, by assumption. □

Next, we consider a further generalization of Theorems 2.3.2 and 2.3.3 to the case of an operator $\mathcal{K}$ with a matrix-valued kernel.

Theorem 2.3.4. *Let $I = [a,b]$ or $I = \mathbb{R}$. Let $\mathcal{K} \in \mathcal{J}_1(L^2(I, \mathbb{C}^k))$. Since $\mathcal{K}$ is also Hilbert-Schmidt, $\exists \boldsymbol{K} \in L^2(I \times I, \mathbb{C}^{k\times k})$ so that*

$$(\mathcal{K}\boldsymbol{\phi})(x) = \int_I \boldsymbol{K}(x,y)\boldsymbol{\phi}(y) dy, \tag{2.107}$$

for $\boldsymbol{\phi} \in L^2(I, \mathbb{C}^k)$. Suppose that $\boldsymbol{K} \in C^0(I \times I, \mathbb{C}^{k\times k})$ and that $F(x) := \operatorname{Tr}(\boldsymbol{K})(x,x) \in L^1(I, \mathbb{C})$. Then

$$\operatorname{Tr}(\mathcal{K}) = \int_I \operatorname{Tr}(\boldsymbol{K})(x,x) dx. \tag{2.108}$$

Proof. Define

$$\left(\mathcal{K}^{\mathrm{Tr}}\phi\right)(x) = \int_I \operatorname{Tr}(\mathbf{K})(x,y)\phi(y) dy \tag{2.109}$$

for $\phi \in L^2(I,\mathbb{C})$. Since $\mathbf{K} \in L^2(I \times I, \mathbb{C}^{k\times k})$, it follows that $\text{Tr}(\mathbf{K}) \in L^2(I \times I, \mathbb{C})$. Consequently, $\mathcal{K}^{\text{Tr}} \in \mathcal{J}_2(L^2(I,\mathbb{C}))$.

Claim:

$$\mathcal{K}^{\text{Tr}} \in \mathcal{J}_1(L^2(I,\mathbb{C})), \tag{2.110}$$

and

$$\text{Tr}(\mathcal{K}) = \text{Tr}\big(\mathcal{K}^{\text{Tr}}\big). \tag{2.111}$$

Since $\mathcal{K}$ is Hilbert-Schmidt, it is compact. So by Theorem 2.1.1,

$$\mathcal{K} = \sum_j \mu_j \langle \boldsymbol{\phi}_j, \cdot \rangle \boldsymbol{\psi}_j. \tag{2.112}$$

Thus,

$$
\begin{aligned}
(\mathcal{K}\boldsymbol{\phi})(x) &= \sum_j \mu_j \langle \boldsymbol{\phi}_j, \boldsymbol{\phi} \rangle_{L^2(I,\mathbb{C}^k)} \boldsymbol{\psi}_j(x) && (2.113)\\
&= \sum_j \mu_j \int_I \boldsymbol{\phi}_j^*(y)\boldsymbol{\phi}(y)dy\, \boldsymbol{\psi}_j(x) && (2.114)\\
&= \int_I \sum_j \mu_j \boldsymbol{\phi}_j^*(y)\boldsymbol{\phi}(y)\boldsymbol{\psi}_j(x)dy && (2.115)\\
&= \int_I \sum_j \mu_j \boldsymbol{\psi}_j(x)\boldsymbol{\phi}_j^*(y)\boldsymbol{\phi}(y)dy && (2.116)\\
&= \int_I \mathbf{K}(x,y)\boldsymbol{\phi}(y)dy, && (2.117)
\end{aligned}
$$

where

$$\mathbf{K}(x,y) = \sum_j \mu_j \boldsymbol{\psi}_j(x)\boldsymbol{\phi}_j(y). \tag{2.118}$$

Then

$$
\begin{aligned}
\mathcal{K}^{\mathrm{Tr}}\phi(x) &:= \int_I \mathrm{Tr}(\mathbf{K})(x,y)\phi(y)dy && (2.119)\\
&= \int_I \sum_j \mu_j \,\mathrm{Tr}\big(\boldsymbol{\psi}_j(x)\boldsymbol{\phi}_j(y)\big)\phi(y)dy && (2.120)\\
&= \int_I \sum_j \mu_j \boldsymbol{\phi}_j^T(y)\boldsymbol{\psi}_j(x)\phi(y)dy && (2.121)\\
&= \int_I \sum_j \sum_{\ell=1}^{k} \phi_{j\ell}(y)\psi_{j\ell}(x)\phi(y)dy && (2.122)\\
&= \sum_{j,\ell} \mu_j \langle \phi_{j\ell}, \phi\rangle \psi_{j\ell}, && (2.123)
\end{aligned}
$$

where

$$
\boldsymbol{\phi}_j = \begin{bmatrix} \phi_{j1} \\ \vdots \\ \phi_{jk} \end{bmatrix}. \tag{2.124}
$$

That is, the compact operator $\mathcal{K}^{\mathrm{Tr}}$ admits a representation as in Theorem 2.1.1, with absolutely convergent singular values

$$
\sum_j |\mu_j| < \infty, \tag{2.125}
$$

so that $\mathcal{K}^{\mathrm{Tr}} \in \mathcal{J}_1$ by definition. Thus, the trace of $\mathcal{K}^{\mathrm{Tr}}$ is defined, and so (2.111) holds. We note by assumption, that $\mathrm{Tr}(\mathbf{K}) \in C^0(I \times I, \mathbb{C})$, since $\mathbf{K} \in C^0(I \times I, \mathbb{C}^{k\times k})$, and that $\mathrm{Tr}(\mathbf{K})(x,x) \in L^1(I,\mathbb{C})$. Hence, the assumptions of the previous two theorems hold for $\mathcal{K}^{\mathrm{Tr}}$. That is, by Theorems 2.3.2 and 2.3.3, we have that

$$
\mathrm{Tr}\big(\mathcal{K}^{\mathrm{Tr}}\big) = \int_I \mathrm{Tr}(\mathbf{K})(x,x)dx, \tag{2.126}
$$

since

$$\operatorname{Tr}(\mathcal{K}) = \sum_{m=1}^{\infty}\sum_{j=1}^{k}\langle \boldsymbol{\phi}_{m,j}, \mathcal{K}\boldsymbol{\phi}_{m,j}\rangle_{L^2(\mathbb{R},\mathbb{C}^k)} \tag{2.127}$$

$$= \sum_{m=1}^{\infty}\sum_{j=1}^{k}\int_I\int_I \left[\boldsymbol{\phi}_{m,j}(x)\right]^T \mathbf{K}(x,y)\boldsymbol{\phi}_{m,j}(y)dxdy \tag{2.128}$$

$$= \sum_{m=1}^{\infty}\int_I\int_I \phi_m(x)\left[\sum_{j=1}^{k}\mathbf{e}_j^T\mathbf{K}(x,y)\mathbf{e}_j\right]\phi_m(y)dxdy \tag{2.129}$$

$$= \sum_{m=1}^{\infty}\int_I\int_I \phi_m(x)\operatorname{Tr}(\mathbf{K})(x,y)\phi_m(y)dxdy \tag{2.130}$$

$$= \sum_{m=1}^{\infty}\langle \phi_m, \mathcal{K}^{\mathrm{Tr}}\phi_m\rangle_{L^2(I,\mathbb{C})}. \tag{2.131}$$

□

We continue to generalize the previous results to calculate the trace of the $n-$th wedge product of a trace class integral operator $\mathcal{K}$, and hence the determinant $\det(\mathcal{I}+\mathcal{K})$.

First, we consider the following hypothesis.

Hypothesis 2.3.5. *The operator $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R},\mathbb{C}^k))$ is of the form*

$$(\mathcal{K}\boldsymbol{\phi})(x) = \int_{\mathbb{R}} \boldsymbol{K}(x,y)\boldsymbol{\phi}(y)dy, \tag{2.132}$$

where $\boldsymbol{\phi} \in L^2(\mathbb{R},\mathbb{C}^k)$ and $\boldsymbol{K} \in C^0(\mathbb{R}\times\mathbb{R},\mathbb{C}^{k\times k}) \cap L^2(\mathbb{R}\times\mathbb{R},\mathbb{C}^{k\times k})$ has the property that $\exists C,a,b>0$ such that

$$\|\boldsymbol{K}(x,y)\|_{\mathbb{C}^{k\times k}} \le Ce^{-a|x|}e^{-b|y|},\ \forall x,y\in\mathbb{R}. \tag{2.133}$$

Theorem 2.3.6. *Let $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R},\mathbb{C}^k))$ satisfy Hypothesis 2.3.5. For each $n\in\mathbb{N}$, let*

$$K_{\boldsymbol{j}}^{(n)}(\boldsymbol{x},\boldsymbol{y}) := \det\left(\left[\boldsymbol{K}_{j_\alpha j_\beta}(x_\alpha,y_\beta)\right]_{\alpha,\beta=1}^{n}\right), \tag{2.134}$$

where $\boldsymbol{x}=(x_1,\ldots,x_n)$, $\boldsymbol{y}=(y_1,\ldots,y_n)$, and

$$\boldsymbol{j}\in J_k^{(n)} = \{(j_1\ldots j_n) : 1\le j_\alpha\le k,\ \forall\alpha\},$$

is an index set of cardinality $|J_k^{(n)}| = k^n$. *Then*

$$\mathrm{Tr}(\wedge^n \mathcal{K}) = \sum_{\boldsymbol{j} \in J_k^{(n)}} \frac{1}{n!} \int_{\mathbb{R}^n} \boldsymbol{K}_{\boldsymbol{j}}^{(n)}(\boldsymbol{x}, \boldsymbol{x}) d\boldsymbol{x}. \tag{2.135}$$

Consequently,

$$\det(\mathcal{I} + z\mathcal{K}) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{\boldsymbol{j} \in J_k^{(n)}} \int_{\mathbb{R}^n} \boldsymbol{K}_{\boldsymbol{j}}^{(n)}(\boldsymbol{x}, \boldsymbol{x}) d\boldsymbol{x}. \tag{2.136}$$

Remark. *To unpack the definition of* $K_{\boldsymbol{j}}^{(n)}(\boldsymbol{x}, \boldsymbol{y})$ *in (2.134), we observe that* $[K_{j_\alpha j_\beta}(x_\alpha, y_\beta)]_{\alpha,\beta=1}^n$ *is the* $n \times n$ *matrix whose* $(\alpha, \beta)-$*entry,* $K_{j_\alpha j_\beta}(x_\alpha, y_\beta)$*, is the* $(j_\alpha, j_\beta)-$*entry of the* $k \times k$ *matrix-valued kernel* K *evaluated at the point* $(x_\alpha, y_\beta) \in \mathbb{R}^2$*. Here,* x_α, y_β *are the* α *and* β *entries of the vectors* $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$*. Therefore the formula for* $\det(\mathcal{I} + z\mathcal{K})$ *in (2.136) is given as an infinite sum over an index* $n \in \mathbb{N}$ *and a multi-index* $\boldsymbol{j} \in J_k^{(n)}$ *of integrals over* $\mathbb{R}^n$ *of determinants of* $n \times n$ *matrices. Needless to say, this formula cannot be used in numerical calculations! However, it will prove to be very useful to establish convergence properties of a numerical approximation to* $\det(\mathcal{I} + z\mathcal{K})$ *that we will derive in a later section. We note the similarities between the determinant formula in (2.134) and the generalized von Koch formula in (2.64), which we will use to approximate Fredholm determinants of operators with matrix-valued kernels on the real line by matrix determinants.*

Proof. First, we establish (2.135) for $\mathrm{Tr}(\wedge^n \mathcal{K})$ over a finite interval I, instead of $\mathbb{R}$. We can assume that $I = [0, 1]$. For each fixed N, let

$$\phi_m(x) = \begin{cases} 2^{N/2}, & \frac{m-1}{2^N} \leq x < \frac{m}{2^N} \\ 0, & \text{otherwise.} \end{cases} \tag{2.137}$$

Then $\{\phi_{m,j} : m = 1, \ldots, 2^N\}$ is an orthonormal set in $L^2([0,1], \mathbb{C})$. Let $\{\mathbf{e}_1, \ldots, \mathbf{e}_k\}$ be the standard basis for $\mathbb{C}^k$. Let

$$\boldsymbol{\phi}_{m,j}(x) := \phi_m(x)\mathbf{e}_j.$$

Then $\{\phi_{m,j} : 1 \le m \le 2^N,\ 1 \le j \le k\}$ is an orthonormal set in $L^2((0,1),\mathbb{C}^k)$. Set

$$\mathbf{\Phi}_{\mathbf{m},\mathbf{j}} = \boldsymbol{\phi}_{m_1,j_1} \wedge \cdots \wedge \boldsymbol{\phi}_{m_n,j_n}, \tag{2.138}$$

and let $\ell = \ell(m,j) = (m-1)k + j$. Then the ordering $\ell_1 < \ell_2$ corresponds to the lexicographic ordering $((m_1,j_1) < (m_2,j_2)) \iff (m_1 < m_2 \text{ or } m_1 = m_2 \text{ and } j_1 < j_2)$. Let $\mathbf{m} = (m_1 \ldots m_n)$ and $\mathbf{j} = (j_1 \ldots j_n)$, and define

$$\mathcal{M}_N^{(n),\uparrow} = \{(\mathbf{m},\mathbf{j}) : (m_1,j_1) < (m_2,j_2) < \cdots < (m_n,j_n) : 1 \le m_\ell \le 2^N, 1 \le j_\ell \le k\}. \tag{2.139}$$

Then $\mathcal{B}_N = \{\mathbf{\Phi}_{\mathbf{m},\mathbf{j}} : (\mathbf{m},\mathbf{j}) \in \mathcal{M}_N^{(n),\uparrow}\}$ is an orthonormal set in $L^2([0,1],\mathbb{C}^k)$. Let $\mathcal{P}_N$ be the projection onto $\operatorname{Span}(\wedge^n \mathcal{B}_N)$. Arguing as in the proof of Theorem 2.3.2, we have that

$$\operatorname{Tr}(\wedge^n \mathcal{K}) = \lim_{N\to\infty} \operatorname{Tr}(\mathcal{P}_N\,(\wedge^n\mathcal{K})\,\mathcal{P}_N) = \frac{1}{n!} \sum_{\mathbf{m}\in\mathcal{M}_N^{(n)}} \sum_{\mathbf{j}\in J_k^{(n)}} \langle \mathbf{\Phi}_{\mathbf{m},\mathbf{j}}, (\wedge^n\mathcal{K})\,\mathbf{\Phi}_{\mathbf{m},\mathbf{j}}\rangle_{\wedge^n L^2(I,\mathbb{C}^k)}, \tag{2.140}$$

where

$$\mathcal{M}_N^{(n)} = \{\mathbf{m} = (m_1 \ldots m_n) : 1 \le m_\alpha \le 2^N,\ \forall\alpha\}, \tag{2.141}$$

$$J_k^{(n)} = \{\mathbf{j} = (j_1 \ldots j_n) : 1 \le j_\alpha \le k,\ \forall\alpha\}. \tag{2.142}$$

In addition, by Lemma 2.3.7 below,

$$\operatorname{Tr}(\mathcal{P}_N(\wedge^n\mathcal{K})\mathcal{P}_N) = \frac{1}{n!} \sum_{\mathbf{m}\in\mathcal{M}_N^{(n)}} \sum_{\mathbf{j}\in J_k^{(n)}} \langle \mathbf{\Phi}_{\mathbf{m},\mathbf{j}}, (\wedge^n\mathcal{K})\,\mathbf{\Phi}_{\mathbf{m},\mathbf{j}}\rangle_{\wedge^n L^2(I,\mathbb{C}^k)}. \tag{2.143}$$

Claim:

$$\langle \phi_{m_\alpha}\mathbf{e}_{j_\alpha}, \mathcal{K}\left(\phi_{m_\beta}\mathbf{e}_{j_\beta}\right)\rangle_{L^2(I,\mathbb{C}^k)} \cong \frac{1}{2^N} K_{j_\alpha j_\beta}\left(\frac{m_\alpha}{2^N}, \frac{m_\beta}{2^N}\right), \tag{2.144}$$

to within an error that approaches 0 as $N \to \infty$.

Proof. We have that

$$\begin{aligned}
\langle \phi_{m_\alpha}\mathbf{e}_{j_\alpha}, \mathcal{K}\left(\phi_{m_\beta}\mathbf{e}_{j_\beta}\right)\rangle_{L^2(I,\mathbb{C}^k)} &= \langle \phi_{m_\alpha}\mathbf{e}_{j_\alpha}, \int_I \sum_{i=1}^{k} K_{ij_\beta}(x,y)\phi_{m_\beta}(y)dy\ \mathbf{e}_i\rangle \\
&= \sum_{i=1}^{k} \iint\limits_{I\times I} \phi_{m_\alpha}(x)(\mathbf{e}_{j_\alpha})^T K_{ij_\beta}(x,y)\phi_{m_\beta}(y)\mathbf{e}_i dxdy \\
&= \iint\limits_{I\times I} \phi_{m_\alpha}(x)\phi_{m_\beta}(y)K_{j_\alpha j_\beta}(x,y)dxdy \\
&= \langle \phi_{m_\alpha}, K_{j_\alpha j_\beta}\phi_{m_\beta}\rangle_{L^2(I,\mathbb{C})} \\
&\cong \frac{1}{2^N}K_{j_\alpha j_\beta}\left(\frac{m_\alpha}{2^N}, \frac{m_\beta}{2^N}\right), \qquad (2.145)
\end{aligned}$$

with an error that converges to zero as $N \to \infty$, for the same reasons as in the proof of Theorem 2.3.2. □

Then by (2.140) and (2.144), and since

$$\langle \psi_1 \wedge \cdots \wedge \psi_n, \phi_1 \wedge \cdots \wedge \phi_n\rangle = \det[\langle \psi_i, \phi_j\rangle]_{i,j=1}^n, \qquad (2.146)$$

we have that

$$\begin{aligned}
\mathrm{Tr}\left(\mathcal{P}_N\left(\wedge^n\mathcal{K}\right)\mathcal{P}_N\right) &\cong \frac{1}{n!}\sum_{\mathbf{m}\in\mathcal{M}_N^{(n)}}\sum_{\mathbf{j}\in J_k^{(n)}} \det\left[\frac{1}{2^N}K_{j_\alpha j_\beta}\left(\frac{m_\alpha}{2^N}, \frac{m_\beta}{2^N}\right)\right]_{\alpha,\beta=1}^n \qquad (2.147) \\
&= \frac{1}{n!}\sum_{\mathbf{m}\in\mathcal{M}_N^{(n)}}\sum_{\mathbf{j}\in J_k^{(n)}} \left(\frac{1}{2^N}\right)^n K_{\mathbf{j}}^{(n)}\left(\frac{m_\alpha}{2^N}, \frac{m_\beta}{2^N}\right) \qquad (2.148) \\
&\cong \frac{1}{n!}\sum_{\mathbf{j}\in J_k^{(n)}} \int_{I^n} K_j^{(n)}(\mathbf{x},\mathbf{x})d\mathbf{x}, \qquad (2.149)
\end{aligned}$$

where the error in (2.149) converges to 0 since (2.148) is a Riemann sum for the continuous function $F^{(n)}(x) := \mathbf{K}_j^{(n)}(\mathbf{x},\mathbf{x})$. This establishes the result in the case that $\mathcal{K} \in \mathcal{J}_1(L^2(I,\mathbb{C}^k))$, where I is a finite interval. To prove (2.136) for operators on $\mathbb{R}$, we first establish the following claim.

Claim: Suppose that $\mathcal{K}$ satisfies Hypothesis 2.3.5. Then $\forall n$, $F^{(n)}(\mathbf{x}) := K^{(n)}(\mathbf{x},\mathbf{x}) \in L^2(\mathbb{R}^n, \mathbb{C})$.

Proof.

$$\begin{aligned} \left|K^{(n)}_{\mathbf{j}}(\mathbf{x},\mathbf{y})\right| &= \left|\det\left[K_{j_\alpha j_\beta}(x_\alpha, y_\beta)\right]_{\alpha,\beta=1}^n\right| && (2.150)\\ &= \left|\sum_{\pi\in\sigma(n)} (-1)^\pi K_{j_1 j_{\pi(1)}}(x_1, y_{\pi(1)}) \dots K_{j_n j_{\pi(n)}}(x_n, y_{\pi(n)})\right| && (2.151)\\ &\le \sum_{\pi\in\sigma(n)} C^n e^{-(\alpha|x_1|+\beta|y_{\pi(1)}|)} \dots e^{-(\alpha|x_n|+\beta|y_{\pi(n)}|)} && (2.152)\\ &= n! C^n e^{-\alpha(|x_1|+\dots+|x_n|)} e^{-\beta(|y_1|+\dots+|y_n|)}, && (2.153) \end{aligned}$$

which immediately implies that $K^{(n)}(\mathbf{x},\mathbf{x}) \in L^1(\mathbb{R}^n, \mathbb{C})$. □

Finally, arguing as in the proof of Theorem 2.3.3, we obtain (2.135) and (2.136). □

In the proof of Theorem 2.3.6 above, we made use of the following lemma, which we prove.

Lemma 2.3.7. *Let $\mathcal{K}$ be a linear operator on a separable Hilbert space $\mathcal{H}$. Fix $N \in \mathbb{N}$, and let $\{\phi_{N,m}(x)\}$ be an orthonormal set in $\mathcal{H}$, chosen so that $\cup_{N=1}^\infty \mathcal{B}_N$ is an orthonormal basis for $\mathcal{H}$. Let*

$$\Phi_{N,\boldsymbol{m}} = \phi_{N,m_1} \wedge \dots \wedge \phi_{N,m_n}, \tag{2.154}$$

where $\boldsymbol{m} = (m_1, \dots, m_n)$, and let

$$\mathcal{M}_N^{(n),\uparrow} = \{\boldsymbol{m} : 1 \le m_1 < \dots < m_n \le N\}. \tag{2.155}$$

Then

$$\wedge^n \mathcal{B}_N = \{\Phi_{\boldsymbol{m}}\}_{\boldsymbol{m}\in\mathcal{M}_N^{(n),\uparrow}} \tag{2.156}$$

is an orthonormal set in $\wedge^n\mathcal{H}$. Let $\mathcal{P}_N$ be the projection onto $\mathrm{Span}(\wedge^n \mathcal{B}_N)$. *Then*

$$\mathrm{Tr}(\mathcal{P}_N \wedge^n \mathcal{K} \mathcal{P}_N) = \frac{1}{n!} \sum_{\boldsymbol{m}\in\mathcal{M}_N^{(n)}} \langle \Phi_{N,\boldsymbol{m}}, \wedge^n \mathcal{K} \Phi_{N,\boldsymbol{m}} \rangle, \tag{2.157}$$

where

$$\mathcal{M}_N^{(n)} = \{\boldsymbol{m} = (m_1 \dots m_n) : 1 \le m_\alpha \le N, \forall \alpha\}. \tag{2.158}$$

Proof. By the definition of the trace,

$$\mathrm{Tr}(\mathcal{P}_N \mathcal{K} \mathcal{P}_N) = \sum_{\mathbf{m} \in \mathcal{M}_N^{(n),\uparrow}} \langle \Phi_{\mathbf{m}}, \wedge^n(\mathcal{K}) \Phi_{\mathbf{m}} \rangle = \frac{1}{n!} \sum_{\mathbf{m} \in \mathcal{M}_N^{(n)}} \langle \Phi_{\mathbf{m}}, \wedge^n \mathcal{K} \Phi_{\mathbf{m}} \rangle. \tag{2.159}$$

To establish (2.157), we argue as follows. If $\mathbf{m}$ has a repeated entry, i.e. $\exists k \neq \ell$, such that $m_k = m_\ell$, then $\Phi_{\mathbf{m}} = 0$ holds. Let

$$\mathcal{M}_N^{(n),0} = \{\mathbf{m} \in \mathcal{M}_N^{(n)} : \exists k \neq \ell : m_k = m_\ell\}. \tag{2.160}$$

Then

$$\mathcal{M}_N^{(n)} \setminus \mathcal{M}_N^{(n),0} = \{\pi(\mathbf{m}) : \mathbf{m} \in \mathcal{M}_N^{(n),\uparrow}, \pi \in \sigma(n)\}. \tag{2.161}$$

Therefore,

$$\sum_{\mathbf{m} \in \mathcal{M}_N^{(n)}} \langle \Phi_{\mathbf{m}}, \wedge^n(\mathcal{K}) \Phi_{\mathbf{m}} \rangle = \sum_{\mathbf{m} \in \mathcal{M}_N^{(n)} \setminus \mathcal{M}_N^{(n),0}} \langle \Phi_{\mathbf{m}}, \wedge^n(\mathcal{K}) \Phi_{\mathbf{m}} \rangle \tag{2.162}$$

$$= \sum_{\mathbf{m} \in \mathcal{M}_N^{(n),\uparrow}} \sum_{\pi \in \sigma(n)} \langle \Phi_{\pi(\mathbf{m})}, \wedge^n(\mathcal{K}) \Phi_{\pi(\mathbf{m})} \rangle. \tag{2.163}$$

Since

$$\Phi_{\pi(\mathbf{m})} = (-1)^\pi \Phi_{\mathbf{m}}, \tag{2.164}$$

we have that

$$\sum_{\mathbf{m} \in \mathcal{M}_N^{(n)}} \langle \Phi_{\mathbf{m}}, \wedge^n(\mathcal{K}) \Phi_{\mathbf{m}} \rangle = \sum_{\mathbf{m} \in \mathcal{M}_N^{(n),\uparrow}} \sum_{\pi \in \sigma(n)} \langle \Phi_{\pi(\mathbf{m})}, \wedge^n(\mathcal{K}) \Phi_{\pi(\mathbf{m})} \rangle \tag{2.165}$$

$$= n! \sum_{\mathbf{m} \in \mathcal{M}_N^{(n),\uparrow}} \langle \Phi_{\mathbf{m}}, \wedge^n(\mathcal{K}) \Phi_{\mathbf{m}} \rangle, \tag{2.166}$$

□

2.3.1 2-Modified Fredholm Determinant

In this subsection, we review the definition and properties of the 2-modified Fredholm determinant of a Hilbert-Schmidt operator. The results in this section summarize and extend those in Simon [24]. First, we generalize Simon's proof of a formula for the $2-$modified Fredholm determinant of a linear operator, $\mathcal{K} \in \mathcal{J}_2(L^2(I, \mathbb{C}))$, on a compact interval with a scalar kernel, to the case of a linear operator, $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^k))$, on the real line with a matrix-valued kernel. Finally, we state and prove a closely related formula for the $2-$modified determinant of a block matrix.

First, we state the following lemma.

Lemma 2.3.8. *[24, Lemma 9.1] Suppose $\mathcal{A} \in \mathcal{J}_2(\mathcal{H})$. Let*

$$R_2(\mathcal{A}) = (1 + \mathcal{A})e^{-\mathcal{A}} - 1. \tag{2.167}$$

Then $R_2(\mathcal{A}) \in \mathcal{J}_1$.

Proof. Let $g(z) := (1 + z)e^{-z} - 1$, and let $h(z) = \frac{g(z)}{z^2}$. Then the power series of h is given by

$$\begin{aligned} h(z) &= \frac{g(z)}{z^2} = \frac{(1+z)e^{-z} - 1}{z^2} \\ &= \frac{(1+z)(1 - z + \frac{z^2}{2} + O(z^3)) - 1}{z^2} \\ &= \frac{\frac{-z^2}{2} + O(z^3)}{z^2} \\ &= \frac{-1}{2} + O(z), \end{aligned} \tag{2.168}$$

meaning that h has a removable singularity at $z = 0$. Since g is an entire function, so is h. Now, for any entire function, h, we have a power series representation

$$h(z) = \sum_{n=0}^{\infty} a_n z^n, \tag{2.169}$$

and since $\mathcal{A}$ is bounded, the operator

$$h(\mathcal{A}) := \sum_{n=0}^{\infty} a_n \mathcal{A}^n \tag{2.170}$$

is defined and also bounded. Now, we have that

$$g(\mathcal{A}) = \mathcal{A}^2 h(\mathcal{A}). \tag{2.171}$$

By assumption, $\mathcal{A} \in \mathcal{J}_2$, so $\mathcal{A}^2 \in \mathcal{J}_1$, since the product of two elements of ℓ_2 is in ℓ_1. Thus,

$$R_2(\mathcal{A}) = g(\mathcal{A}) \in \mathcal{J}_1, \tag{2.172}$$

as $\mathcal{J}_1(\mathcal{H})$ is an ideal in $\mathcal{B}(\mathcal{H})$. $\square$

The 2-modified Fredholm determinant of a Hilbert-Schmidt operator is defined as follows.

Definition 2.3.9. *[24, pg. 75] Let $\mathcal{A} \in \mathcal{J}_2(\mathcal{H})$. Then we define*

$$\det_2(\mathcal{I} + \mathcal{A}) := \det(1 + R_2(\mathcal{A})) = \det\left((1 + \mathcal{A})e^{-\mathcal{A}}\right). \tag{2.173}$$

Theorem 2.3.10. *[24, Theorem 9.2] Let $\mathcal{A}, \mathcal{B} \in \mathcal{J}_2(\mathcal{H})$. Then*

1. $\det_2(\mathcal{I} + \mathcal{A}) = \prod_{k=1}^{N(\mathcal{A})} \left[(1 + \lambda_k(\mathcal{A}))e^{-\lambda_k(\mathcal{A})}\right]$,

2. $|\det_2(\mathcal{I} + \mathcal{A})| \leq \exp(\Gamma_2 \|\mathcal{A}\|_2^2)$, *for some constant* Γ,

3. $|\det_2(\mathcal{I} + \mathcal{A}) - \det_2(\mathcal{I} + \mathcal{B})| \leq \|\mathcal{A} - \mathcal{B}\|_2 \exp(\Gamma(\|\mathcal{A}\|_2 + \|\mathcal{B}\|_2 + 1)^2)$,

4. *If $\mathcal{A} \in \mathcal{J}_1$, then*

$$\det_2(\mathcal{I} + \mathcal{A}) = \det(\mathcal{I} + \mathcal{A})e^{-\operatorname{Tr}(\mathcal{A})}, \tag{2.174}$$

   and

5. *$\mathcal{I} + \mathcal{A}$ is invertible if and only if* $\det_2(\mathcal{I} + \mathcal{A}) \neq 0$.

Proof. (1) First note that since g is an entire function, it follows from the spectral mapping theorem [33] that

$$\lambda_k(g(\mathcal{A})) = g(\lambda_k(\mathcal{A})), \tag{2.175}$$

where $\{\lambda_k(\mathcal{A})\}_{k=1}^{N(\mathcal{A})}$ are the eigenvalues of $\mathcal{A}$. Thus we have that

$$\begin{aligned}
\det{}_2(\mathcal{I}+\mathcal{A}) &= \det(1+g(\mathcal{A})) \\
&= \prod_{k=1}^{N(\mathcal{A})}(1+\lambda_k(g(\mathcal{A}))), \text{ since } g(\mathcal{A}) \in \mathcal{J}_1 \\
&= \prod_{k=1}^{N(\mathcal{A})}(1+g(\lambda_k(\mathcal{A}))) \\
&= \prod_{k=1}^{N(\mathcal{A})}\left[(1+\lambda_k(\mathcal{A}))e^{-\lambda_k(\mathcal{A})}\right]. \qquad (2.176)
\end{aligned}$$

(4) If $\mathcal{A} \in \mathcal{J}_1$, then by (1),

$$\begin{aligned}
\det{}_2(\mathcal{I}+\mathcal{A}) &= \prod_{k=1}^{N(\mathcal{A})}[(1+\lambda_k(\mathcal{A}))e^{-\lambda_k(\mathcal{A})}] \\
&= \prod_{k=1}^{N(\mathcal{A})}[1+\lambda_k(\mathcal{A})]\prod_{k=1}^{N(\mathcal{A})}e^{-\lambda_k(\mathcal{A})} \\
&= \det(\mathcal{I}+\mathcal{A})e^{-\sum\lambda_k(\mathcal{A})} \\
&= \det(\mathcal{I}+\mathcal{A})e^{-\operatorname{Tr}(\mathcal{A})}. \qquad (2.177)
\end{aligned}$$

(5)

$$\begin{aligned}
\det{}_2(\mathcal{I}+\mathcal{A}) &= \det(1+R_2(\mathcal{A})) \neq 0 \\
&\Longleftrightarrow (\mathcal{I}+R_2(\mathcal{A})) = (\mathcal{I}+\mathcal{A})e^{-\mathcal{A}} \text{ is invertible} \\
&\Longleftrightarrow (\mathcal{I}+\mathcal{A}) \text{ is invertible.}
\end{aligned}$$

The proofs of (2) and (3) can be found in [24]. □

Proposition 2.3.11. *Assume that both $\mathcal{AB}, \mathcal{BA} \in \mathcal{J}_2(\mathcal{H})$, where $\mathcal{A}$ and $\mathcal{B}$ are bounded linear operators on $\mathcal{H}$. Then*

$$\det{}_2(\mathcal{I}+\mathcal{AB}) = \det{}_2(\mathcal{I}+\mathcal{BA}). \qquad (2.178)$$

Proof. By Theorem 2 in Deift [34], the spectra of $\mathcal{AB}$ and $\mathcal{BA}$ are identical, including multiplicity, away from 0. Since $\mathcal{AB} \in \mathcal{J}_2(\mathcal{H})$, by Theorem 2.3.10, we have

$$\det_2(\mathcal{I} + \mathcal{AB}) = \prod_{k=1}^{N(\mathcal{AB})} \left[(1 + \lambda_k(\mathcal{AB}))e^{-\lambda_k(\mathcal{AB})}\right], \tag{2.179}$$

and if $\lambda = 0$ is an eigenvalue of either $\mathcal{AB}$ or $\mathcal{BA}$, then

$$(1 + \lambda)e^{-\lambda} = 1, \tag{2.180}$$

so $\det_2(\mathcal{I} + \mathcal{AB}) = \det_2(\mathcal{I} + \mathcal{BA})$

□

Next we adapt the results of Theorem 2.3.6 to the case of the 2-modified determinant. We will see that the results are extremely similar, with only a slight change in the format of the integrands. We start by generalizing a result from [24], in which we derive the von Koch formula for the 2-modified Fredholm determinant of a Hilbert-Schmidt operator with a matrix-valued kernel.

Theorem 2.3.12. *[24] Let I be a finite interval, and let $\mathcal{K} \in \mathcal{J}_2(L^2(I, \mathbb{C}))$ be of the form*

$$\mathcal{K}\phi(x) = \int_I K(x, y)\phi(y)dy. \tag{2.181}$$

Then

$$\det_2(\mathcal{I} + \mathcal{K}) = \sum_{n=0}^{\infty} \frac{\int_{I^n} \widetilde{K}(\boldsymbol{x}, \boldsymbol{x})d\boldsymbol{x}}{n!}, \tag{2.182}$$

where $\boldsymbol{x} = (x_1 \ldots x_n)$, and

$$\widetilde{K}(\boldsymbol{x}, \boldsymbol{x}) := \det\left([K(x_i, x_j)[1 - \delta_{ij}]]_{i,j=1}^n\right). \tag{2.183}$$

We do not include the proof of this theorem, as it is almost identical to the proof of the following, more general theorem, in which we evaluate the $2-$modified Fredholm determinant of a Hilbert-Schmidt operator with a matrix-valued kernel on the real line.

Theorem 2.3.13. *Let $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^k))$ satisfy Hypothesis 2.3.5. Let $\widetilde{K}_{\boldsymbol{j}}^{(n)} : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{C}$ be the $n \times n$ determinant defined by*

$$\widetilde{K}_{\boldsymbol{j}}^{(n)}(\boldsymbol{x}, \boldsymbol{y}) := \det\left[K_{j_\alpha j_\beta}(x_\alpha, y_\beta)[1 - \delta_{\alpha\beta}]\right]_{\alpha,\beta=1}^{n}, \tag{2.184}$$

where

$$\boldsymbol{x} = (x_1, \ldots, x_n), \tag{2.185}$$

$$\boldsymbol{y} = (y_1, \ldots, y_n), \tag{2.186}$$

and $K_{ij}(x, y)$ is the $(i, j)-$element of the matrix-valued kernel of the operator $\mathcal{K}$. Here,

$$\boldsymbol{j} \in J_k^{(n)} = \{(j_1 \ldots j_n) : 1 \leq j_\alpha \leq k,\ \forall \alpha\}. \tag{2.187}$$

Then

$$\det{}_2(\mathcal{I} + \mathcal{K}) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\boldsymbol{j} \in J_k^{(n)}} \int_{\mathbb{R}^n} \widetilde{K}_{\boldsymbol{j}}^{(n)}(\boldsymbol{x}, \boldsymbol{x}) d\boldsymbol{x}. \tag{2.188}$$

Proof. Since any $\mathcal{K} \in \mathcal{J}_2$ is compact, $\mathcal{K}$ is the limit of finite rank operators which, in particular, are in $\mathcal{J}_1$. So by the continuity of $\det_2$ given in (3) of Theorem 2.3.10, it suffices to prove the result for $\mathcal{K} \in \mathcal{J}_1$. For fixed n and fixed $\mathbf{j} \in J_k^{(n)}$, let

$$\alpha_{\mathbf{j}}^{(n)}(\lambda) := \int_{\mathbb{R}^n} K_{\mathbf{j}}^{(n)}(\mathbf{x}, \mathbf{x}; \lambda) d\mathbf{x}, \tag{2.189}$$

where

$$K_{\mathbf{j}}^{(n)}(\mathbf{x}, \mathbf{x}; \lambda) = \det\left[K_{j_\alpha j_\beta}(x_\alpha, x_\beta)(1 - \lambda\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^{n}. \tag{2.190}$$

Let $F : \mathbb{C} \to \mathbb{C}$ be defined by

$$F(\lambda) = \sum_{n=0}^{\infty} \sum_{\mathbf{j} \in J_k^{(n)}} \frac{\alpha_{\mathbf{j}}^{(n)}(\lambda)}{n!}. \tag{2.191}$$

Then we know that

$$\det(\mathcal{I} + \mathcal{K}) = F(0), \tag{2.192}$$

and we want to show that

$$\det{}_2(\mathcal{I}+\mathcal{K}) = F(1), \tag{2.193}$$

Now, for $\mathcal{K} \in \mathcal{J}_1$, we have that

$$\det{}_2(\mathcal{I}+\mathcal{K}) = \det(\mathcal{I}+\mathcal{K})e^{-\operatorname{Tr}(\mathcal{K})}, \tag{2.194}$$

so we need to prove that

$$F(\lambda) = F(0)e^{-\lambda \operatorname{Tr}(\mathcal{A})}, \tag{2.195}$$

since this will imply that

$$\sum_{n=0}^{\infty} \sum_{\mathbf{j} \in J_k^{(n)}} \frac{\alpha_{\mathbf{j}}^{(n)}(1)}{n!} = F(1) = \det(\mathcal{I}+\mathcal{K})e^{-\operatorname{Tr}(\mathcal{K})} = \det{}_2(\mathcal{I}+\mathcal{K}), \tag{2.196}$$

as required. The result (2.195) will follow once we know that

$$F'(\lambda) = -\operatorname{Tr}(\mathcal{K})F(\lambda), \tag{2.197}$$

due to the uniqueness to solutions of ODE's. Now,

$$\frac{\partial \alpha_{\mathbf{j}}^{(n)}}{\partial \lambda}(\lambda) = \int_{\mathbb{R}^n} \frac{\partial}{\partial \lambda} \det\left[K_{j_\alpha j_\beta}(x_\alpha, x_\beta)(1-\lambda\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^{n} d\mathbf{x}. \tag{2.198}$$

Let $\mathbf{B}_{\mathbf{j}}(\lambda)$ be the $n \times n$ matrix defined by

$$[\mathbf{B}_{\mathbf{j}}(\lambda)]_{\alpha\beta} = [K(x_\alpha, x_\beta)]_{j_\alpha j_\beta}[1-\lambda\delta_{\alpha\beta}]. \tag{2.199}$$

Then $\det \circ \mathbf{B}_{\mathbf{j}} : \mathbb{R} \to \mathbb{C}^{n\times n} \to \mathbb{C}$ maps $\lambda \mapsto \mathbf{B}_{\mathbf{j}}(\lambda) \mapsto \det(\mathbf{B}_{\mathbf{j}}(\lambda))$. By the chain rule,

$$\frac{d}{d\lambda}(\det \circ \mathbf{B}_{\mathbf{j}})(\lambda) = \sum_{\alpha,\beta=1}^{n} \frac{\partial(\det \mathbf{B}_{\mathbf{j}})}{\partial b_{\alpha\beta}} \frac{\partial b_{\alpha\beta}}{\partial \lambda}, \tag{2.200}$$

where $b_{\alpha\beta} = [\mathbf{B}_{\mathbf{j}}(\lambda)]_{\alpha\beta}$. Let $\mathbf{B}_{\mathbf{j}}^{(\alpha,\beta)}$ be the $(n-1)\times(n-1)$ matrix obtained by removing row α and column β from $\mathbf{B}_{\mathbf{j}}$. By the cofactor expansion of the determinant [35],

$$\frac{\partial}{\partial b_{\alpha\alpha}} \det(\mathbf{B}_{\mathbf{j}}) = \det \mathbf{B}_{\mathbf{j}}^{(\alpha,\alpha)}. \tag{2.201}$$

Since λ only appears on the diagonal, $\frac{\partial b_{\alpha\beta}}{\partial\lambda} = 0$ for $\alpha \neq \beta$, and so

$$\frac{d}{d\lambda}(\det \circ \mathbf{B_j})(\lambda) = \sum_{\alpha=1}^{n} \frac{\partial(\det \mathbf{B_j})}{\partial b_{\alpha\alpha}} \frac{\partial b_{\alpha\alpha}}{\partial\lambda} = -\sum_{\alpha=1}^{n} \det \mathbf{B}_{\mathbf{j}}^{(\alpha,\alpha)} K_{j_\alpha j_\alpha}(x_\alpha, x_\alpha). \tag{2.202}$$

Since $\mathbf{B}_{\mathbf{j}}^{(\alpha,\alpha)}$ does not include x_α, and $\mathbf{K}(x_\alpha, x_\alpha)$ only involves x_α, we find that

$$\sum_{\mathbf{j}\in J_k^{(n)}} \frac{\partial\alpha_{\mathbf{j}}^{(n)}}{\partial\lambda}(\lambda) = -\sum_{\mathbf{j}\in J_k^{(n)}} \int_{\mathbb{R}^{n-1}} K_{\mathbf{j}}^{(n-1)}(\mathbf{x},\mathbf{x};\lambda)d\mathbf{x} \sum_{\alpha=1}^{n} \int_I K_{j_\alpha j_\alpha}(x_\alpha, x_\alpha)dx_\alpha. \tag{2.203}$$

Now, for fixed n, and for each $\alpha \in \{1, \ldots, n\}$, we have a bijection P_α between index sets given by

$$P_\alpha \left(J_k^{(n-1)} \times J_k^{(1)}\right) \to J_k^{(n)}, \tag{2.204}$$

which maps $((j_1, j_2, \ldots, j_{\alpha-1}, j_\alpha, \ldots, j_{n-1}), \beta) \mapsto (j_1, \ldots, j_{\alpha-1}, \beta, j_\alpha, \ldots, j_{n-1})$. Using this bijection, we have that

$$\begin{aligned}
\frac{d}{d\lambda}F(\lambda) &= \sum_{n=0}^{\infty} \sum_{\mathbf{j}\in J_k^{(n)}} \frac{\partial}{\partial\lambda}\alpha_{\mathbf{j}}^{(n)}(\lambda) \\
&= -\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\mathbf{j}\in J_k^{(n-1)}} \left[\int_{\mathbb{R}^{n-1}} K_{\mathbf{j}}^{(n-1)}(\mathbf{x},\mathbf{x};\lambda)d\mathbf{x}\right] \sum_{\alpha=1}^{n} \int_{\mathbb{R}} K_{j_\alpha j_\alpha}(x_\alpha, x_\alpha)dx_\alpha \\
&= -\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\alpha=1}^{n} \left(\sum_{\mathbf{j}\in J_k^{(n-1)}} \alpha_{\mathbf{j}}^{(n-1)}(\lambda) \int_{\mathbb{R}} \sum_{j_\alpha=1}^{k} K_{j_\alpha j_\alpha}(x,x)dx \right) \\
&= -\sum_{n=0}^{\infty} \frac{1}{n!} \left(\sum_{\mathbf{j}\in J_k^{(n-1)}} \alpha_{\mathbf{j}}^{(n-1)}(\lambda) \right) \sum_{\alpha=1}^{n} \int_{\mathbb{R}} \operatorname{Tr}(\mathbf{K})(x,x)dx \\
&= -n \operatorname{Tr}(\mathcal{K}) \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\mathbf{j}\in J_k^{(n-1)}} \alpha_{\mathbf{j}}^{(n-1)}(\lambda) \\
&= -\operatorname{Tr}(\mathcal{K}) \sum_{n=1}^{\infty} \sum_{\mathbf{j}\in J_k^{(n-1)}} \frac{\alpha_{\mathbf{j}}^{(n)}(\lambda)}{(n-1)!} \\
&= -\operatorname{Tr}(\mathcal{K}) \sum_{n=0}^{\infty} \sum_{\mathbf{j}\in J_k^{(n)}} \frac{\alpha_{\mathbf{j}}^{(n)}(\lambda)}{n!} \\
&= -\operatorname{Tr}(\mathcal{K})F(\lambda),
\end{aligned} \tag{2.205}$$

as required. $\square$

Finally, we state and prove a von-Koch formula for the 2-modified Fredholm determinant of a block matrix. We recall from (2.58) and (2.59) that an $M\times M$ block matrix, $\mathbf{K}$, with $k\times k$ blocks defines a linear operator $\mathcal{K} : L(I_M, \mathbb{C}^k) \to L(I_M, \mathbb{C}^k)$, where $I_M = \{1, 2, \ldots, M\}$. Since all linear operators on finite-dimensional spaces are Hilbert-Schmidt, $\mathcal{K}$ has a $2-$modified Fredholm determinant, which by Theorem 2.3.13 is given by

$$\det{}_2(\mathcal{I}+\mathcal{K}) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \int_{I^n} \widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x},\mathbf{x})d\mathbf{x}, \tag{2.206}$$

for $\widetilde{K}_{\mathbf{j}}^{(n)}$ as defined in (2.184) and $J_k^{(n)}$ as in (2.187). In analogy with the von-Koch formula given in Theorem 2.2.1 for the regular determinant of a block matrix, and with the formula for the $2-$modified determinant of a Hilbert-Schmidt operator on $L^2(\mathbb{R}, \mathbb{C}^k)$ given in Theorem 2.3.13, we have the follow result.

Theorem 2.3.14. *Let $\boldsymbol{K} \in \mathbb{C}^{kM\times kM}$ be an $M \times M$ block matrix of $k \times k$ blocks, given by*

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{K}(1,1)\ldots & \boldsymbol{K}(1,M) \\ \vdots & \vdots \\ \boldsymbol{K}(M,1)\ldots & \boldsymbol{K}(M,M) \end{bmatrix}, \tag{2.207}$$

where each $\boldsymbol{K}(m_1, m_2)$ is a $k \times k$ matrix. For each n, let

$$J_k^{(n)} = \{\boldsymbol{j} = (j_1, j_2, \ldots, j_n) : 1 \le j_\alpha \le k,\ \forall\ \alpha\}, \tag{2.208}$$

$$\mathcal{M}_M^{(n)} = \{\boldsymbol{m} = (m_1, m_2, \ldots, m_n) : 1 \le m_\alpha \le M,\ \forall\ \alpha\}, \tag{2.209}$$

and define

$$K_{\boldsymbol{j}}^{(n)}(\boldsymbol{m}) := \det\left[[\boldsymbol{K}(m_\alpha, m_\beta)]_{j_\alpha j_\beta}(1-\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^{n} \tag{2.210}$$

for each $\boldsymbol{j} \in J_k^{(n)}$ and $\boldsymbol{m} \in \mathcal{M}_M^{(n)}$. Then

$$\det{}_2(\boldsymbol{I}+\boldsymbol{K}) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\boldsymbol{j}\in J_k^{(n)}} \sum_{\boldsymbol{m}\in\mathcal{M}_M^{(n)}} K_{\boldsymbol{j}}^{(n)}(\boldsymbol{m}). \tag{2.211}$$

Remark. *The proof of this result is basically the same as the proof of Theorem 2.3.13, provided that* $K_{\boldsymbol{j}}^{(n)}(\boldsymbol{x},\boldsymbol{x};\lambda)$ *is replaced by*

$$K_{\boldsymbol{j}}^{(n)}(\boldsymbol{m};\lambda) = \det\left([\boldsymbol{K}(m_\alpha, m_\beta)]_{j_\alpha j_\beta}[1-\lambda\delta_{\alpha\beta}]\right)_{\alpha,\beta=1}^{n} \tag{2.212}$$

and $\int_{\mathbb{R}^n}\cdot$ *by* $\sum_{\boldsymbol{m}\in\mathcal{M}_M^{(n)}}\cdot$. *Nevertheless, for the sake of completeness, we include the proof.*

Proof. Since $\mathbf{K}$ is a finite matrix, it is necessarily trace class. Therefore, by (2.174), it should be that

$$\det{}_2(\mathbf{I}+\mathbf{K}) = \det(\mathbf{I}+\mathbf{K})e^{-\operatorname{Tr}(\mathbf{K})}. \tag{2.213}$$

So, we define a function $F(\lambda)$ such that $F(0)=\det(\mathbf{I}+\mathbf{K})$, and $F(1)=\det_2(\mathbf{I}+\mathbf{K})$, and we show that

$$F(\lambda) = F(0)e^{-\lambda Tr(\mathbf{K})}, \tag{2.214}$$

which will imply that

$$F(1) = \det(\mathbf{I}+\mathbf{K})e^{-\operatorname{Tr}(\mathbf{K})}. \tag{2.215}$$

We define

$$F(\lambda) = \sum_{n=0}^{\infty}\sum_{\mathbf{j}\in J_k^{(n)}}\frac{\alpha_{\mathbf{j}}^{(n)}(\lambda)}{n!}, \tag{2.216}$$

where for fixed n and fixed $\mathbf{j}\in J_k^{(n)}$,

$$\alpha_{\mathbf{j}}^{(n)}(\lambda) := \sum_{j_1,\ldots,j_n=1}^{k}\sum_{m_1,\ldots,m_n=1}^{M}K_{\mathbf{j}}^{(n)}(\mathbf{m};\lambda) \tag{2.217}$$

with

$$K_{\mathbf{j}}^{(n)}(\mathbf{m};\lambda) := \det\left(\left[\mathbf{K}(m_\alpha,m_\beta)\right]_{j_\alpha j_\beta}[1-\lambda\delta_{\alpha\beta}]\right]_{\alpha,\beta=1}^{n}\right). \tag{2.218}$$

Then (2.214) will follow when we show that

$$F'(\lambda) = -\operatorname{Tr}(\mathbf{K})F(\lambda), \tag{2.219}$$

where $\mathrm{Tr}(\mathbf{K})$ is the trace of the $kM \times kM$ matrix $\mathbf{K}$. Let

$$[\mathbf{B}_{\mathbf{j},\mathbf{m}}(\lambda)]_{\alpha\beta} := [\mathbf{K}(m_\alpha, m_\beta)]_{j_\alpha j_\beta}(1 - \lambda\delta_{\alpha\beta}). \tag{2.220}$$

Then

$$\frac{\partial}{\partial\lambda}(\det \circ \mathbf{B}_{\mathbf{j},\mathbf{m}})(\lambda) = \sum_{\alpha,\beta=1}^{n} \frac{\partial \mathbf{B}_{\mathbf{j},\mathbf{m}}}{\partial b_{\alpha\beta}} \frac{\partial b_{\alpha\beta}}{\partial\lambda}. \tag{2.221}$$

Let $\mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\beta)}$ be the $(n-1)\times(n-1)$ matrix obtained by removing row α and column β from $\mathbf{B}_{\mathbf{j},\mathbf{m}}$. Now,

$$\frac{\partial}{\partial b_{\alpha\alpha}}(\det \circ \mathbf{B}_{\mathbf{j},\mathbf{m}}) = \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)}, \tag{2.222}$$

and since $\frac{\partial b_{\alpha\beta}}{\partial\lambda} = 0$ for $\alpha \neq \beta$, we have that

$$\frac{\partial}{\partial\lambda}(\det \circ \mathbf{B}_{\mathbf{j},\mathbf{m}}) = -\sum_{\alpha=1}^{n} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)} K_{j_\alpha j_\alpha}(x_{m_\alpha}, x_{m_\alpha}). \tag{2.223}$$

Thus

$$\frac{\partial \alpha_{n,\mathbf{j}}}{\partial\lambda} = -\sum_{\mathbf{m}\in\mathcal{M}_N^{(n)}} \sum_{\alpha=1}^{n} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)} K_{j_\alpha j_\alpha}(x_{m_\alpha}, x_{m_\alpha}). \tag{2.224}$$

We note that since $\mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)}$ does not depend on x_{m_α},

$$\sum_{\alpha=1}^{n} \sum_{\mathbf{m}\in\mathcal{M}_N^{(n)}} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)} K_{j_\alpha j_\alpha}(x_{m_\alpha}, x_{m_\alpha}) = \sum_{\alpha=1}^{n} \sum_{m_1,\ldots,\cancel{m_\alpha},\ldots,m_n=1}^{N} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{\alpha,\alpha} \sum_{m_\alpha=1}^{N} K_{j_\alpha j_\alpha}(x_{m_\alpha}, x_{m_\alpha}). \tag{2.225}$$

Arguing as in the proof of Theorem 2.3.13, we have that

$$F'(\lambda) = -\sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\alpha=1}^{n} \sum_{\mathbf{j}\in J_k^{(n-1)}} \left[\sum_{m_1,\ldots,\cancel{m_\alpha},m_n=1}^{M} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)} \sum_{m_\alpha=1}^{M} [\mathbf{K}(m_\alpha, m_\beta)]_{j_\alpha j_\beta} \right]. \tag{2.226}$$

Now, for fixed n, and for each $\alpha \in \{1, \ldots, n\}$, we have the bijection

$$P_\alpha \left(J_k^{(n-1)} \times J_k^{(1)} \right) \to J_k^{(n)} \tag{2.227}$$

given by

$$((j_1, j_2, \ldots, \cancel{j_\alpha}, \ldots, j_{n-1}), j_\alpha) \mapsto (j_1, \ldots, j_\alpha, \ldots, j_{n-1}). \tag{2.228}$$

Therefore,

$$\sum_{j_1,\ldots,j_\alpha,\ldots,j_n=1}^{k} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(\alpha,\alpha)}[\mathbf{K}(m_\alpha,m_\beta)]_{j_\alpha j_\beta} = \sum_{j_1,\ldots,j_{n-1}=1}^{k} \det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(n-1)} \sum_{j_\alpha=1}^{k}[\mathbf{K}(m_\alpha,m_\beta)]_{j_\alpha j_\beta}, \quad (2.229)$$

where $\mathbf{B}_{\mathbf{j},\mathbf{m}}^{(n-1)}$ is the $(n-1)\times(n-1)$ matrix associated with $\mathbf{B}_{\mathbf{j},\mathbf{m}}$. Then by (2.225) and (2.229), we have that

$$\begin{aligned}
F'(\lambda) &= -\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\alpha=1}^{n}\sum_{\mathbf{j}\in J_k^{(n-1)}}\sum_{\mathbf{m}\in\mathcal{M}_k^{(n-1)}}\det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(n-1)}\sum_{j_\alpha=1}^{k}\sum_{m_\alpha=1}^{N}[\mathbf{K}(m_\alpha,m_\beta)]_{j_\alpha j_\beta} \\
&= -\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\mathbf{j}\in J_k^{(n-1)}}\sum_{\mathbf{m}\in\mathcal{M}_k^{(n-1)}}\det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(n-1)}\sum_{\alpha=1}^{n}\left[\sum_{j_\alpha=1}^{k}\sum_{m_\alpha=1}^{N}[\mathbf{K}(m_\alpha,m_\beta)]_{j_\alpha j_\beta}\right] \\
&= -\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\mathbf{j}\in J_k^{(n-1)}}\sum_{\mathbf{m}\in\mathcal{M}_k^{(n-1)}}\det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(n-1)}\left(\sum_{\alpha=1}^{n}\mathrm{Tr}(\mathbf{K})\right) \\
&= -(n\,\mathrm{Tr}\,\mathbf{K})\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\mathbf{j}\in J_k^{(n-1)}}\sum_{\mathbf{m}\in\mathcal{M}_k^{(n-1)}}\det \mathbf{B}_{\mathbf{j},\mathbf{m}}^{(n-1)} \\
&= -n\,\mathrm{Tr}\,\mathbf{K}\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\mathbf{j}\in J_k^{(n-1)}}\alpha_{\mathbf{j}}^{(n-1)}(\lambda). \qquad (2.230)
\end{aligned}$$

Then re-indexing gives

$$\begin{aligned}
\frac{d}{d\lambda}F(\lambda) &= -\mathrm{Tr}(\mathbf{K})\sum_{n=0}^{\infty}\frac{n}{n!}\sum_{\mathbf{j}\in J_k^{n-1}}\alpha_{\mathbf{j}}^{(n-1)}(\lambda) \\
&= -\mathrm{Tr}(\mathbf{K})\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\sum_{\mathbf{j}\in J_k^{(n-1)}}\alpha_{\mathbf{j}}^{(n-1)}(\lambda) \\
&= -\mathrm{Tr}(\mathbf{K})\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}\alpha_{\mathbf{j}}^{(n)}(\lambda) \\
&= -\mathrm{Tr}(\mathbf{K})F(\lambda), \qquad (2.231)
\end{aligned}$$

as required. □

2.4 Truncation Error

Because the Fredholm determinant in (2.188) is in the form of an infinite sum, with integrals over all of $\mathbb{R}^n$, it is not practical to calculate. Instead, we must numerically approximate $\det_2(\mathcal{I}+\mathcal{K})$, and to do so, we proceed as follows. First, we truncate $\mathbb{R}^n$ to the finite interval $[-L, L]^n$, which will yield a truncation error. Then, we must evaluate the integrals over $[-L, L]^n$ using a numerical quadrature rule, which will yield an additional quadrature error. In this manner, the Fredholm determinant can be approximated by a block-matrix determinant, which is easy to compute. Then, the error between our approximated determinant and the true determinant, $\det_2(\mathcal{I}+\mathcal{K})$, will be less than the sum of the truncation and quadrature errors. If, in addition, our kernel is trace class, the same error bounds will apply due to the similarity in formulae for $\det_2$ and $\det_1$. Following the work of Bornemann [26], we prove results about the convergence of these truncation and quadrature errors in the case where $\mathcal{K}$ has a matrix-valued kernel. Additionally, we quantify the rate of convergence of these errors, assuming the exponential decay of the kernel. The proofs of these results rely on the similarity between the formula for the Fredholm determinants given in Theorems 2.3.6 and 2.3.13 on the one hand, and on the generalized von-Koch formulae for $\det_p(\mathbf{I}+z\mathbf{K})$, for $p = 1$ and 2, given in Theorems 2.2.1 and 2.3.14, on the other hand.

Remark. *Let $\mathcal{K} \in \mathcal{J}_p(L^2(\mathbb{R}, \mathbb{C}^k))$, for $p = 1$ or 2, and define*

$$\mathcal{K}|_{[-L,L]} := P_L \circ \mathcal{K} \circ \iota_L, \tag{2.232}$$

where $\iota_L : L^2([-L, L], \mathbb{C}^k) \to L^2(\mathbb{R}, \mathbb{C}^k)$ is a bounded inclusion operator, and $P_L : L^2(\mathbb{R}, \mathbb{C}^k) \to L^2([-L, L], \mathbb{C}^k)$ is the bounded projection operator

$$(P_L\boldsymbol{\psi})(x) = \chi_{[-L,L]}(x)\boldsymbol{\psi}(x), \tag{2.233}$$

with $\chi_{[-L,L]}$ being the characteristic function of $[-L, L]$. Since $\mathcal{J}_p$ is an ideal, $\mathcal{K}|_{[-L,L]} \in \mathcal{J}_p(L^2([-L, L], \mathbb{C}^k))$.

Definition 2.4.1. *We say that a sequence of operators, $\{P_n\}$, on a Hilbert space $\mathcal{H}$* converges strongly *to the identity $\mathcal{I}$ if*

$$\|P_n(v) - v\|_{\mathcal{H}} \to 0, \ \forall v \in \mathcal{H}. \tag{2.234}$$

If, in addition, $\mathcal{K} \in \mathcal{J}_1$, then by a similar argument, $\mathcal{K}|_{[-L,L]} \in \mathcal{J}_1$.

Proposition 2.4.2. *If $\mathcal{K} \in \mathcal{J}_p$, for $p = 1$ or 2, and if each of $P_n \circ \mathcal{K} \to \mathcal{K}$ strongly in $\mathcal{J}_p$ norm, then*

$$\det_p(\mathcal{I} + P_n \circ \mathcal{K}) \to \det_p(\mathcal{I} + \mathcal{K}). \tag{2.235}$$

Similarly, if $\mathcal{K} \circ Q_n \to \mathcal{K}$ strongly in $\mathcal{J}_p$, then

$$\det_p(\mathcal{I} + \mathcal{K} \circ Q_n) \to \det_p(\mathcal{I} + \mathcal{K}). \tag{2.236}$$

Remark. *By the proposition, $\det_p(\mathcal{I} + \mathcal{K}|_{[-L,L]}) \to \det_p(\mathcal{I} + \mathcal{K})$ as $L \to \infty$. The following result, which is useful when performing numerical computations, provides an estimate on the rate of convergence.*

Theorem 2.4.3. *Let $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^k))$, be given by*

$$(\mathcal{K}\boldsymbol{\phi})(x) = \int_{\mathbb{R}} \boldsymbol{K}(x,y)\boldsymbol{\phi}(y)dy. \tag{2.237}$$

Define $\mathcal{K}|_{[-L,L]}$ by

$$(\mathcal{K}|_{[-L,L]}\boldsymbol{\phi})(x) = \int_{-L}^{L} \mathbf{K}(x,y)\boldsymbol{\phi}(y)dy. \tag{2.238}$$

Then $\mathcal{K}|_{[-L,L]} \in \mathcal{J}_p(L^2([-L,L], \mathbb{C}^k))$. Additionally assume that $\exists\, C, a > 0$ such that

$$|\boldsymbol{K}_{ij}(x,y)| \le Ce^{-a(|x|+|y|)}, \ \forall i,j \in \{1,...,k\}, \forall x,y, \in \mathbb{R}. \tag{2.239}$$

Then

$$\left|\det_p(\mathcal{I} + z\mathcal{K}) - \det_p(\mathcal{I} + z\mathcal{K}|_{[-L,L]})\right| \le e^{-aL}\boldsymbol{\Phi}\left(\frac{2Ckz}{a}\right), \tag{2.240}$$

where

$$\boldsymbol{\Phi}(\eta) = \sum_{n=1}^{\infty} \frac{n^{(n+2)/n}}{n!}\eta^n. \tag{2.241}$$

Remark. *In Chapter 3, we will show that when $\boldsymbol{K}$ is C^1 off the diagonal, and additionally satisfies the exponential decay condition given in (2.239), where its first partial derivatives satisfy the same exponential decay condition, then $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R}, \mathbb{C}^k))$, and similarly, $\mathcal{K}|_{[-L,L]} \in \mathcal{J}_1(L^2([-L,L], \mathbb{C}^k))$.*

Proof. For each $n \in \mathbb{N}$, let

$$J_k^{(n)} = \{\mathbf{j} = (j_1, \ldots, j_n) : 1 \leq j_\alpha \leq k, \forall \alpha\}, \tag{2.242}$$

and define for $\mathcal{K} \in \mathcal{J}_p$, $p = 1$ or 2,

$$\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}, \mathbf{y}) := \det \left[K_{j_\alpha j_\beta}(x_\alpha, y_\beta)(1 - (p-1)\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^{n}, \tag{2.243}$$

where $K_{j_\alpha j_\beta}(x_\alpha, y_\beta)$ denotes the $(j_\alpha, j_\beta)-$entry of the $k \times k$ matrix-valued kernel $\mathbf{K}(x_\alpha, y_\beta)$. Then, by Theorems 2.3.12 and 2.3.13,

$$\det{}_p(\mathcal{I} + z\mathcal{K}|_{[-L,L]}) = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\mathbf{j} \in J_k^{(n)}} \int_{[-L,L]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}, \mathbf{x}) d\mathbf{x}. \tag{2.244}$$

The error between true and truncated determinants is given by

$$E_L := |\det{}_p(\mathcal{I} + z\mathcal{K}) - \det{}_p(\mathcal{I} + z\mathcal{K}|_{[-L,L]})| \leq \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\mathbf{j} \in J_k^{(n)}} \int_{\mathbb{R}^n \setminus [-L,L]^n} |\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}, \mathbf{x})| d\mathbf{x}. \tag{2.245}$$

To estimate the determinant in (2.243), we apply Hadamard's inequality, which says that if $\mathbf{A} \in \mathbb{C}^{n \times n}$, then

$$|\det(\mathbf{A})| \leq \prod_{\beta=1}^{n} \|\mathbf{A}_{*\beta}\|_2, \tag{2.246}$$

where $\mathbf{A}_{*,\beta}$ denotes the $\beta-$th column of $\mathbf{A}$. Geometrically, this inequality states that the volume of the $n-$dimensional parallelipiped is less than or equal to the product of the lengths of its edges. Thus, we have for both $p = 1$ and $p = 2$ that

$$|\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}, \mathbf{x})| \leq \prod_{\beta=1}^{n} \|\mathbf{A}_{*\beta}\|_2, \tag{2.247}$$

where

$$\mathbf{A}_{*\beta} = \begin{bmatrix} K_{j_1 j_\beta}(x_1, x_\beta) \\ \vdots \\ K_{j_n j_\beta}(x_n, x_\beta) \end{bmatrix}. \tag{2.248}$$

Now, by the assumption in (2.239),

$$\begin{aligned} \|\mathbf{A}_{*\beta}\|_2^2 &= |K_{j_1 j_\beta}(x_1, x_\beta)|^2 + \cdots + |K_{j_n j_\beta}(x_n, x_\beta)|^2 \\ &\leq C^2 \left[e^{-2a(|x_1|+|x_\beta|)} + \cdots + e^{-2a(|x_n|+|x_\beta|)}\right] \\ &= C^2 e^{-2a|x_\beta|} \left[e^{-2a|x_1|} + \cdots + e^{-2a|x_n|}\right] \\ &\leq nC^2 e^{-2a|x_\beta|}, \end{aligned} \tag{2.249}$$

where the final inequality follows from the fact that $e^{-a|x|} < 1$ for $a > 0$. Therefore,

$$|\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x})| \leq C^n n^{n/2} e^{-a\|\mathbf{x}\|_1}, \tag{2.250}$$

and so, using the fact that $|J_k^{(n)}| = k^n$, we have that

$$|E_L| \leq \sum_{n=1}^{\infty} \frac{z^n}{n!} (Ck)^n n^{n/2} \int_{\mathbb{R}^n \setminus [-L,L])^n} e^{-a\|\mathbf{x}\|_1} d\mathbf{x}. \tag{2.251}$$

Let us consider the $n-$dimensional integral in (2.251). When $n = 2$,

$$\mathbb{R}^2 \setminus [-L, L]^2 = \{|x_1| > L\} \cup \{|x_2| > L\}, \tag{2.252}$$

although this union is not disjoint. Therefore,

$$\begin{aligned} \int\limits_{\mathbb{R}^2 \setminus [-L,L]^2} e^{-a(|x_1|+|x_2|)} dx_1 dx_2 &\leq \int\limits_{|x_1|>L} dx_1 \int_{-\infty}^{\infty} e^{-a(|x_1|+|x_2|)} dx_2 + \int\limits_{|x_2|>L} dx_2 \int_{-\infty}^{\infty} e^{-a(|x_1|+|x_2|)} dx_1 \\ &= 2 \left(\int_{|x|>L} e^{-a|x|} dx \right) \left(\int_{\mathbb{R}} e^{-a|x|} \right). \end{aligned} \tag{2.253}$$

Now,

$$\begin{aligned} \int_{|x|>L} e^{-a|x|} dx &= \int_{-\infty}^{-L} e^{ax} dx + \int_L^{\infty} e^{-ax} dx \\ &= \frac{1}{a} \left[e^{-aL} - \lim_{x \to -\infty} e^{ax} \right] + \frac{-1}{a} \left[\lim_{x \to \infty} e^{-ax} - e^{-aL} \right] \\ &= \frac{2}{a} e^{-aL}, \end{aligned} \tag{2.254}$$

and similarly,

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-a|x|}dx &= \int_{-\infty}^{0} e^{ax}dx + \int_{0}^{\infty} e^{-ax}dx \\ &= \frac{1}{a}\left[1 - \lim_{x\to-\infty} e^{ax}\right] + \frac{-1}{a}\left[\lim_{x\to\infty} e^{-ax} - 1\right] \\ &= \frac{2}{a}. \end{aligned} \tag{2.255}$$

Therefore,

$$\int\limits_{\mathbb{R}^2\setminus[-L,L]^2} e^{-a(|x_1|+|x_2|)}dx_1dx_2 \le 2\left(\frac{2}{a}e^{-aL}\right)\left(\frac{2}{a}\right). \tag{2.256}$$

Similarly, for $n = 3$, let $I_3 = \int\limits_{\mathbb{R}^3\setminus[-L,L]^3} e^{-a(|x_1|+|x_2|+|x_3|)}dx_1dx_2dx_3$. Then

$$\begin{aligned} I_3 &\le \int\limits_{|x_3|>L}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a(|x_1|+|x_2|+|x_3|)}dx_1dx_2dx_3 \\ &\quad + \int\limits_{|x_2|>L}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a(|x_1|+|x_2|+|x_3|)}dx_1dx_3dx_2 \\ &\quad + \int\limits_{|x_1|>L}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a(|x_1|+|x_2|+|x_3|)}dx_2dx_3dx_1 \\ &= 3\left(\frac{2}{a}e^{-aL}\right)\left(\frac{2}{a}\right)^2. \end{aligned} \tag{2.257}$$

Iteratively, we can see that if $I_n = \int_{\mathbb{R}^n\setminus[-L,L]^n} e^{-a\|\mathbf{x}\|_1}d\mathbf{x}$, then

$$I_n \le n\left(\frac{2}{a}\right)^n e^{-aL}, \tag{2.258}$$

and so by (2.250),

$$\begin{aligned} |E_L| &\le \sum_{n=1}^{\infty}\frac{z^n}{n!}\left(\frac{2Ck}{a}\right)^n n^{(n+2)/n}e^{-aL} \\ &= e^{-aL}\sum_{n=1}^{\infty}\left(\frac{2zCk}{a}\right)^n\frac{n^{(n+2)/n}}{n!} \\ &= e^{-aL}\mathbf{\Phi}\left(\frac{2zCk}{a}\right), \end{aligned} \tag{2.259}$$

where

$$\boldsymbol{\Phi}(\zeta) = \sum_{n=1}^{\infty} \frac{n^{(n+2)/2}}{n!}\zeta^n. \tag{2.260}$$

□

Note: Bornemann [26] shows that

$$\boldsymbol{\Phi}(z) \leq z\boldsymbol{\Psi}(z\sqrt{2}e), \tag{2.261}$$

where

$$\boldsymbol{\Psi}(z) = 1 + \frac{\sqrt{\pi}}{2} z e^{z^2/4}\left[1 + \operatorname{erf}\left(\frac{z}{2}\right)\right], \tag{2.262}$$

so that the term $\boldsymbol{\Phi}\left(\frac{2zCk}{a}\right)$ in the truncation error estimate

$$|\det_p(\mathcal{I} + z\mathcal{K}) - \det_p(\mathcal{I} + z\mathcal{K}|_{[-L,L]})| \leq e^{-aL}\boldsymbol{\Phi}\left(\frac{2zCk}{a}\right). \tag{2.263}$$

is bounded above by a computable constant depending on the decay of the kernel $\mathbf{K}$.

2.5 Quadrature Method and Error

In order to compute $\det_p(\mathcal{I} + z\mathcal{K}|_{[-L,L]})$, for $p = 1$ or 2, we must approximate the integrals $\int_{[-L,L]^n} \widetilde{K}_{\mathbf{j}}^{(n)} d\mathbf{x}$ using a numerical integration scheme. To do so, we use a quadrature rule based on the composite Simpson's rule and obtain an associated quadrature error. In Theorem 2.5.3 below, we will show that if the kernel $\mathbf{K}$ is Lipschitz-continuous, then the error is $O(\Delta x)$, where Δx is the grid spacing in the quadrature rule.

Let $\mathcal{K} \in \mathcal{J}_2(L^2([a,b], \mathbb{C}^k))$ be a Hilbert-Schmidt operator with a matrix-valued kernel $\mathbf{K} \in (C^0 \cap L^2)([a,b] \times [a,b], \mathbb{C}^{k\times k})$ so that

$$(\mathcal{K}\boldsymbol{\phi})(x) = \int_a^b \mathbf{K}(x,y)\boldsymbol{\phi}(y)dy. \tag{2.264}$$

Let

$$d_2(z) := \det{}_2(\mathcal{I} + z\mathcal{K}), \tag{2.265}$$

for $z \in \mathbb{C}$, be the 2-modified Fredholm determinant of $\mathcal{K}$. If, in addition, $\mathcal{K} \in \mathcal{J}_1(L^2([a,b],\mathbb{C}^k))$ is trace class, then we let

$$d_1(z) := \det(\mathcal{I} + z\mathcal{K}) \tag{2.266}$$

denote the regular Fredholm determinant of $\mathcal{K}$. In this section, we define matrix determinant approximations of (2.265) and (2.266).

Let $Q = Q_M$ be a quadrature rule for functions $f : [a,b] \to \mathbb{C}$ of the form

$$Q_M(f) = \sum_{i=1}^{M} w_i f(x_i), \tag{2.267}$$

that is defined in terms of M nodes $a \le x_1 < x_2 < \cdots < x_M \le b$ and positive weights $w_1, \ldots, w_M$. We suppose that Q_M is a family of quadrature rules that converges for continuous functions, i.e. that

$$Q_M(f) \to \int_a^b f(x)dx, \quad \text{as } M \to \infty, \tag{2.268}$$

for all $f \in C^0([a,b],\mathbb{C})$. We define $\mathbf{K}_Q \in \mathbb{C}^{kM\times kM}$ to be the $M \times M$ block matrix

$$\mathbf{K}_Q = \begin{bmatrix} w_1\mathbf{K}(1,1) & w_2\mathbf{K}(1,2) & \ldots & w_M\mathbf{K}(1,M) \\ w_1\mathbf{K}(2,1) & w_2\mathbf{K}(\mathbf{2,2}) & \ldots & w_M\mathbf{K}(2,M) \\ \vdots & & & \vdots \\ w_1\mathbf{K}(M,1) & w_2\mathbf{K}(M,2) & \ldots & w_M\mathbf{K}(M,M) \end{bmatrix}, \tag{2.269}$$

where

$$\mathbf{K}(\alpha,\beta) := \mathbf{K}(x_\alpha, x_\beta) \in \mathbb{C}^{k\times k} \tag{2.270}$$

is the $k \times k$ matrix obtained by evaluating the matrix-valued kernel $\mathbf{K}$ defined in (2.264), at nodes $x_\alpha, x_\beta \in \{x_i\}_{i=1}^M$ of quadrature rule Q_M. Then the matrix determinant approximation of the $2-$modified Fredholm determinant in (2.265) is defined by

$$d_{2,Q_M}(z) := \det[\mathbf{I}_{kM\times kM} + z\mathbf{K}_Q]e^{-z\,\mathrm{Tr}\left(\mathbf{K}_Q\right)}, \tag{2.271}$$

and the matrix determinant approximation of the regular Fredholm determinant in (2.266) is defined by

$$d_{1,Q_M}(x) = \det[\mathbf{I}_{kM\times kM} + z\mathbf{K}_Q]. \tag{2.272}$$

With some additional assumptions on the kernel $\mathbf{K}$, we can quantify the convergence of the quadrature approximation $d_{p,Q}(z)$ to the Fredholm determinant $d_2p(z)$.

Following [26, Theorem 6.1], we have the following result.

Theorem 2.5.1. *Suppose that $\mathcal{K} \in \mathcal{J}_2(L^2([a,b],\mathbb{C}^k))$ is a Hilbert-Schmidt operator with continuous matrix-valued kernel $\boldsymbol{K} \in C^0([a,b]\times[a,b],\mathbb{C}^{k\times k})$ and that Q_M is a family of quadrature rules on $[a,b]$ that converges for continuous functions. Then*

$$d_{2,Q_M}(z) \to d_2(z) \quad \text{as } M \to \infty \tag{2.273}$$

uniformly in z. If, in addition, $\mathcal{K} \in \mathcal{J}_1(L^2([a,b],\mathbb{C}^k))$, then

$$d_{1,Q_M}(z) \to d_1(z) \quad \text{as } M \to \infty \tag{2.274}$$

uniformly in z.

Remark. *Theorem 3.1.1 in the following chapter will show that if the kernel $\boldsymbol{K}$ is C^0 on $[a,b]\times[a,b]$ and is C^1 away from the diagonal, then $\mathcal{K}$ is trace class on $[a,b]$.*

Proof. For each $n \in \mathbb{N}$, let

$$J_k^{(n)} = \{\mathbf{j} = (j_1,\ldots,j_n) : 1 \le j_\alpha \le k, \forall\alpha\}, \tag{2.275}$$

and define for $p = 1$ or 2,

$$\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x},\mathbf{y}) := \det\left[K_{j_\alpha j_\beta}(x_\alpha, y_\beta)(1-(p-1)\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^{n}, \tag{2.276}$$

where $K_{j_\alpha j_\beta}$ denotes the $(j_\alpha, j_\beta)-$entry of the $k\times k$ matrix-valued kernel, $\mathbf{K}$, in (2.264). Then, by Theorem 2.3.13, for $p = 1, 2$,

$$\det{}_p(\mathcal{I} + z\mathcal{K}) = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x},\mathbf{x})d\mathbf{x}. \tag{2.277}$$

To relate the Fredholm determinant in (2.277) to a matrix determinant, we need to approximate the integral on the right-hand side of (2.277) using an $n-$dimensional quadrature rule. To that end, we recall that by iterated integration, the 1-dimensional quadrature rule, Q_M, can be used to defined the $n-$dimensional quadrature rule $Q^{(n)} = Q_M^{(n)}$ by

$$Q_M^{(n)}(f) := \sum_{\mathbf{m}\in\mathcal{M}_M^{(n)}} w_{m_1}\dots w_{m_M} f(x_{m_1},\dots,x_{m_M}), \tag{2.278}$$

where

$$\mathcal{M}_M^{(n)} = \{\mathbf{m} = (m_1,\dots,m_n) : 1 \le m_\alpha \le M,\ \forall\alpha\}. \tag{2.279}$$

Then since Q_M converges for continuous functions, so does $Q_M^{(n)}$, i.e.,

$$Q_M^{(n)}(f) \to \int_{[a,b]^n} f(\mathbf{x})d\mathbf{x} \tag{2.280}$$

for all $f \in C^0([a,b]^n,\mathbb{C})$. Then letting

$$\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}) := \widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x},\mathbf{x}) \tag{2.281}$$

in (2.277) and calculating formally without regard for convergence issues, we have that for large M,

$$\det{}_p(\mathcal{I} + z\mathcal{K}) \approx 1 + \sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}} Q_M^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}). \tag{2.282}$$

Then by (2.278), (2.276), the multilinearity property of determinants, and (2.270), we obtain

$$\begin{aligned}
d_p(z) &\approx 1 + \sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}\sum_{\mathbf{m}\in\mathcal{M}_M^{(n)}} w_{m_1}\dots w_{m_M}\det\left[\mathbf{K}_{j_\alpha j_\beta}(x_{m_\alpha},x_{m_\beta})(1-(p-1)\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^n \\
&= 1 + \sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}\sum_{\mathbf{m}\in\mathcal{M}_M^{(n)}} \det\left[w_{m_\alpha}\mathbf{K}_{j_\alpha j_\beta}(x_{m_\alpha},x_{m_\beta})(1-(p-1)\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^n \\
&= 1 + \sum_{n=1}^{\infty}\frac{z^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}\sum_{\mathbf{m}\in\mathcal{M}_M^{(n)}} \det\left[[w_{m_\alpha}\mathbf{K}(x_{m_\alpha},x_{m_\beta})]_{j_\alpha j_\beta}(1-(p-1)\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^n \\
&= \det{}_p(\mathbf{I} + z\mathbf{K}_Q) \\
&= d_{p,Q}(z),
\end{aligned} \tag{2.283}$$

where last equality comes from (2.271) and (2.272), following the von-Koch formula (2.211) for the Fredholm determinant of a block matrix.

To rigorously prove that $d_{p,Q_M}(z) \to d_p(z)$ as $M \to \infty$ uniformly in z, we slightly extend the proof in Bornemann [26, Theorem 6.1], for scalar-valued kernels to the case of matrix-valued kernels, which involves the additional sum over $\mathbf{j} \in J_k^{(n)}$ in (2.282). By (2.282) and (2.283),

$$d_{p,Q}(z) - d_p(z) = \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \left(Q^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}) - \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}) d\mathbf{x} \right). \tag{2.284}$$

Let $|z| \leq R$ and choose $\epsilon > 0$. For any $N \in \mathbb{N}$, we can split the series (2.284), as

$$\begin{aligned} |d_{p,Q_M}(z) - d_p(z)| \leq & \sum_{n=1}^{N} \frac{R^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \left| Q_M^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}) - \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(x_1,\dots,x_n) dx_1 \dots dx_n \right| \\ & + \sum_{n=N+1}^{\infty} \frac{R^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \left| Q_M^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}) - \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(x_1,\dots,x_n) dx_1 \dots dx_n \right| \end{aligned} \tag{2.285}$$

Let $\|Q_M\| := \sum_{j=1}^{M} |w_j|$ be the norm of Q_M. We recall from Theorem A.1 of [26] that if a family, Q_M, if quadrature rules converges for continuous functions, then there exists $\Lambda < \infty$ such that $\|Q_M\| < \Lambda$ for all M. Consequently, by (2.278),

$$\|Q_M^{(n)}(f)\| \leq \Lambda^n \|f\|_{L^\infty([a,b]^n,\mathbb{C})}. \tag{2.286}$$

Then we have the bound

$$\begin{aligned} E_{N+1} \;:=\; & \sum_{n=N+1}^{\infty} \frac{R^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \left| Q_M^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}) - \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(x_1,\dots,x_n) dx_1 \dots dx_n \right| \\ \leq\; & \sum_{n=N+1}^{\infty} \frac{R^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \left(\left| Q_M^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}) \right| + \left| \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(x_1,\dots,x_n) dx_1 \dots dx_n \right| \right) \\ \leq\; & \sum_{n=N+1}^{\infty} \sum_{\mathbf{j}\in J_k^{(n)}} \frac{R^n}{n!} (\Lambda^n + (b-a)^n) \|\widetilde{K}_{\mathbf{j}}^{(n)}\|_{L^\infty} \\ \leq\; & \sum_{n=N+1}^{\infty} \sum_{\mathbf{j}\in J_k^{(n)}} \frac{R^n}{n!} 2(\Lambda_1)^n \|\widetilde{K}_{\mathbf{j}}^{(n)}\|_{L^\infty}, \end{aligned} \tag{2.287}$$

where $\Lambda_1 = \max\{\Lambda, b-a\}$. Since the kernel $\mathbf{K}$ is continuous,

$$\|\mathbf{K}\|_{L^\infty([a,b]\times[a,b],\mathbb{C}^{k\times k})} := \max_{1\leq i,j\leq k} \|K_{ij}\|_{L^\infty([a,b]\times[a,b],\mathbb{C})} < \infty. \tag{2.288}$$

Now, as in Lemma A.4 of [26], and by Hadarmard's inequality [35], we have

$$\|\widetilde{K}^{(n)}_{\mathbf{j}}\|_{L^\infty([a,b]^n,\mathbb{C})} \leq n^{n/2}\|\mathbf{K}\|^n_{L^\infty([a,b]\times[a,b],\mathbb{C}^{k\times k})}. \tag{2.289}$$

In addition, since $|J^{(n)}_k| = k^n$, we have that

$$E_{N+1} \leq 2\sum_{n=N+1}^{\infty} \frac{n^{n/2}}{n!}(Rk\Lambda_1\|\mathbf{K}\|_{L^\infty([a,b]\times[a,b],\mathbb{C}^{k\times k})})^n. \tag{2.290}$$

Now as in Lemma A.5 of [26], the series

$$\mathbf{\Phi}(z) = \sum_{n=1}^{\infty} \frac{n^{n/2}}{n!} z^n \tag{2.291}$$

is uniformly absolutely convergent on $|z| < R$. Consequently, we can choose N so that the tail E_{N+1} satisfies

$$E_{N+1} \leq \epsilon/2. \tag{2.292}$$

Given this N, we can choose M_0 so that for all $M > M_0$, the first term in (2.285) is also less than $\epsilon/2$. Given this N, we can choose M_0 so that for all $M > M_0$, the first term in (2.285) is also less than $\epsilon/2$, as required. □

Now, we recall that a function f is Hölder $\alpha-$continuous ($0 < \alpha \leq 1$), $f \in C^{0,\alpha}([a,b],\mathbb{C})$, if

$$|f|_{\mathcal{C}^{0,\alpha}} = \sup_{\mathbf{x}\neq\mathbf{y}\in\mathbb{R}^n} \frac{\|f(\mathbf{x}) - f(\mathbf{y})\|}{\|\mathbf{x}-\mathbf{y}\|^\alpha} < \infty. \tag{2.293}$$

A function f is in the Hölder space $\mathcal{C}^{p,\alpha}([a,b],\mathbb{C})$, for integer $p \geq 0$, if all of its p^{th} partial derivatives are Hölder $\alpha-$continuous. In the special case where $\alpha = 1$, f is Lipschitz-continuous. Assume that the function $f \in C^{p,1}([a,b],\mathbb{C})$. Then the p^{th} derivative $f^{(p)}$ is Lipschitz continuous and so is differentiable almost everywhere with bounded derivative. So

$$\|f^{(p)}\|_{L^\infty[a,b]} = \sup_{x\in[a,b]} |f^{(p)}(x)| < \infty. \tag{2.294}$$

Assuming that our kernel function is at least Lipschitz, we get further bounds on the error between the numerically approximated determinant and the true determinant evaluated on $[a, b]$. We say that a quadrature rule Q is of order ν_Q if $Q(f)$ is exact for all polynomials f up to degree $\nu_Q - 1$. By Theorem A.2 in [26], if $f \in \mathcal{C}^{p-1,1}([a, b])$, then for each one-dimensional quadrature rule Q of order $\nu_Q \geq p$ with positive weights,

$$\left| Q(f) - \int_{[a,b]} f(x)dx \right| \leq c_p(b-a)^{p+1}\nu_Q^{-p}\|f^{(p)}\|_{L^\infty([a,b])}, \tag{2.295}$$

where c_p is a constant depending only on p. In particular, we can choose $c_p = 2\left(\frac{\pi e}{4}\right)^p/\sqrt{2\pi p}$.

Bornemann [26, Theorem A.3] extended the error estimate to the $n-$dimensional quadrature rule $Q^{(n)}(f)$, to obtain

$$\left| Q^{(n)}(f) - \int_{[a,b]^n} f(x_1, \ldots, x_n \right| \leq c_p(b-a)^{n+p}\nu_Q^{-p}\|f^{(p)}\|_{L^\infty([a,b]^n)}. \tag{2.296}$$

This result shows that the quadrature error decays like ν_Q^{-p} as the order, ν_Q, of the quadrature rule increases, $\nu_Q \to \infty$. This error estimate is useful in situations where f is approximated by a single high-degree polynomial on the entire interval $[a, b]$. However, in many situations in numerical analysis, it is more practical to separately approximate f by a low degree polynomial on each interval $[x_i, x_{i+1}]$ and then sum over i to obtain a composite quadrature rule. For such a composite rule, we are interested in the rate at which the quadrature error goes to zero as $\Delta x \to 0$. Bornemann's error estimate (2.296) cannot be applied to composite quadrature rules. Instead, here we show how to derive an error estimate for the $n-$dimensional quadrature rule that is based on the composite Simpson's rule, which is of order $\nu_Q = 4$.

Suppose that $f : [a, b] \to \mathbb{C}$. To derive the composite Simpson's rule, we discretize the interval $[a, b]$ using $2M$ subintervals of width $\Delta x = \frac{b-a}{2M}$, with endpoints at the nodes, $a = x_1 < x_2 < \cdots < x_{2M+1} = b$. Let $I_j = [x_{2j-1}, x_{2j+1}]$ for $i = 1, \ldots, M$, and observe that

$[a,b] = \cup_{j=1}^{M} I_j$. On each subinterval, I_j, we can apply the Simpson's quadrature rule, defined by

$$Q_{I_j}(f) := \sum_{k=-1}^{1} w_k f(x_{2j-k}) \approx \int_{I_j} f(x)dx, \tag{2.297}$$

where $w_{-1} = w_{+1} = \frac{\Delta x}{3}$, and $w_0 = \frac{4\Delta x}{3}$. By (2.295), if $f \in C^{p-1,1}([a,b], \mathbb{C})$, then

$$\left| Q_{I_j}(f) - \int_{I_j} f(x)dx \right| \leq c_p (\Delta x)^{p+1} 4^{-p} \|f^{(p)}\|_{L^\infty(I_j)}. \tag{2.298}$$

Then the composite Simpson's rule is given by

$$Q_{[a,b]}(f) := \sum_{j=1}^{M} Q_{I_j}(f) \approx \int_a^b f(x)dx, \tag{2.299}$$

and by (2.298),

$$\left| Q_{[a,b]}(f) - \int_a^b f(x)dx \right| \leq \frac{1}{2} c_p (b-a)(\Delta x)^p 4^{-p} \|f^{(p)}\|_{L^\infty[a,b]}. \tag{2.300}$$

We observe that

$$Q_{[a,b]}(f) = \sum_{k=1}^{2M+1} w_k f(x_k), \tag{2.301}$$

where now $w_1 = w_{2M+1} = \frac{\Delta x}{3}, w_{2j} = \frac{4\Delta x}{3}$, and $w_{2j+1} = \frac{2\Delta x}{3}$ for $j = 1, \ldots, M-1$.

Theorem 2.5.2. *Suppose that $f \in C^{p-1,1}([a,b]^n)$ for some $p \leq 4$. Let $Q_{[a,b]}^{(n)}$ be the $n-$dimensional quadrature rule induced by the composite Simpson's quadrature rule $Q_{[a,b]}$ in (2.301). Then*

$$\left| \int_{[a,b]^n} f(\boldsymbol{x}) d\boldsymbol{x} - Q_{[a,b]}^{(n)}(f) \right| \leq c_p (b-a)^n 4^{-p} (\Delta x)^p \|f^{(p)}\|_{L^\infty}. \tag{2.302}$$

Proof. Since $[a,b] = \cup_{j=1}^{M} I_j$, we have that

$$[a,b]^n = \bigcup_{j_1,\ldots,j_n=1}^{M} I_{j_1} \times \cdots \times I_{j_n}. \tag{2.303}$$

Therefore,

$$Q_{[a,b]}^{(n)}(f) = \sum_{j_1,\ldots,j_n=1}^{M} Q_{j_1 \ldots j_n}(f), \tag{2.304}$$

where

$$Q_{j_1\dots j_n}(f) = \sum_{k_1,\dots,k_n=-1}^{1} w_{k_1}\dots w_{k_n} f(x_{2j_1-k_1},\dots,x_{2j_n-k_n}) \cong \int_{I_{j_1}\times\cdots\times I_{j_n}} f(x_1,\dots,x_n)dx_1\dots dx_n. \tag{2.305}$$

Let $m \le n$, and let

$$F_{j_1\dots j_m}(y_{m+1},\dots,y_n) := \int_{I_{j_1}\times\cdots\times I_{j_m}} f(x_1,\dots,x_m,y_{m+1},\dots,y_n)dx_1\dots dx_m \tag{2.306}$$

be the partial iterated integral of f, which is approximated by the partial quadrature rule

$$(Q_{j_1\dots j_m}f)(y_{m+1},\dots,y_n) = \sum_{k_1,\dots,k_m=-1}^{1} w_{k_1}\dots w_{k_m} f(x_{2j_1-k_1},\dots,x_{2j_m-k_m},y_{m+1},\dots,y_n) \cong F_{j_1\dots j_m}(y_{m+1},\dots,y_n). \tag{2.307}$$

The identity

$$Q_{j_1\dots j_n}(f) = \sum_{k_1,\dots,k_n=-1}^{1} w_{k_1}\dots w_{k_n} f(x_{2j_1-k_1},\dots,x_{2j_n-k_n}) = \sum_{k_n=-1}^{1} w_{k_n}(Q_{j_1\dots j_{n-1}}f)(x_{2j_n-k_n}) \tag{2.308}$$

enables us to use an induction argument to establish the following claim.

Claim: $\exists A_n \le 2^n$ such that

$$\left|\int_{I_{j_1}\times\cdots\times I_{j_n}} f(x_1,\dots,x_n)dx_1\dots dx_n - Q_{j_1\dots j_n}(f)\right| \le A_n c_p(\Delta x)^{n+p}4^{-p}\|f^{(p)}\|_{L^\infty(I_{j_1}\times\cdots\times I_{j_n})}. \tag{2.309}$$

Proof. By (2.298), $A_1 = 1$ holds. We prove (2.309) by induction on n, by observing that

$$\begin{aligned}
\left|\int_{I_{j_1}\times\cdots\times I_{j_n}} f(\mathbf{x})d\mathbf{x} - Q_{j_1\cdots j_n}(f)\right| &= \left|\int_{I_{j_n}}\int_{I_{j_1}\times\cdots\times I_{j_{n-1}}} f(\mathbf{x},x_n)d\mathbf{x}dx_n - Q_{j_n}(Q_{j_1,\ldots,j_{n-1}}f)\right| \\
&\leq \int_{I_{j_n}}\left|\int_{I_{j_1}\times\cdots\times I_{j_{n-1}}} f(\mathbf{x},x_n)d\mathbf{x} - (Q_{j_1,\ldots,j_{n-1}}f)(x_n)\right| dx_n \\
&\quad + \left|\int_{I_{j_n}} (Q_{j_1\cdots j_{n-1}}f)(x_n)dx_n - Q_{I_{j_n}}(Q_{j_1,\ldots,j_{n-1}}f)\right| \\
&\leq \int_{I_{j_n}} \left[A_{n-1}c_p(\Delta x)^{p+(n-1)}4^{-p}\|f^{(p)}\|_{L^\infty}\right] dx_n \\
&\quad + A_1 c_p(\Delta x)^{p+1}4^{-p}\|(Q_{j_1\cdots j_{n-1}}f)^{(p)}\|_{L^\infty} \\
&\leq A_{n-1}c_p(\Delta x)^{p+n}4^{-p}\|f^{(p)}\|_{L^\infty} \\
&\quad + A_1 c_p(\Delta x)^{p+1}4^{-p}\|(Q_{j_n\cdots j_{n-1}}f)^{(p)}\|_{L^\infty} \\
&\leq \left[A_{n-1} + 2^{n-1}A_1\right](\Delta x)^{n+p}c_p 4^{-p}\|f^{(p)}\|_{L^\infty}, \qquad (2.310)
\end{aligned}$$

since

$$\begin{aligned}
\left|(Q_{j_1\cdots j_{n-1}}f^{(p)})(x_n)\right| &\leq \sum_{k_1,\ldots,k_{n-1}=-1}^{1} w_{k_1}\ldots w_{k_{n-1}}\left|f^{(p)}(x_{2j_1-k_1},\ldots,x_{2j_{n-1}-k_{n-1}},x_n)\right| \\
&\leq (w_{-1}+w_0+w_1)^{n-1}\|f^{(p)}\|_{L^\infty} \\
&= (2\Delta x)^{n-1}\|f^{(p)}\|_{L^\infty}. \qquad (2.311)
\end{aligned}$$

Therefore, $A_n = A_{n-1} + 2^{n-1}$ holds, and so $A_n = 2^n - 1 \leq 2^n$. □

To complete the proof of the Theorem, we observe that by (2.304) and (2.309),

$$\begin{aligned}
\left|\int_{[a,b]^n} f(\mathbf{x})d\mathbf{x} - Q^{(n)}_{[a,b]}f\right| &\leq \sum_{j_1\cdots j_n=1}^{M}\left|\int_{I_{j_1}\times\cdots\times I_{j_n}} f(\mathbf{x})d\mathbf{x} - Q_{j_1\cdots j_n}f\right| \\
&\leq M^n c_p 2^n(\Delta x)^{n+p}4^{-p}\|f^{(p)}\|_{L^\infty([a,b]^n)} \\
&= c_p\left(\frac{b-a}{2\Delta x}\right)^n c_p(2\Delta x)^n(\Delta x)^p 4^{-p}\|f^{(p)}\|_{L^\infty} \\
&= c_p(b-a)^n(\Delta x)^p 4^{-p}\|f^{(p)}\|_{L^\infty}. \qquad (2.312)
\end{aligned}$$

□

Given a matrix-valued kernel $\mathbf{K}$ on $[a,b]$, define

$$\|\mathbf{K}\|_{W^{1,\infty}} = \max\{\|\partial_x \mathbf{K}\|_{L^\infty([a,b]^2,\mathbb{C}^{k\times k})}, \|\partial_y \mathbf{K}\|_{L^\infty([a,b]^2,\mathbb{C}^{k\times k})}, \|\mathbf{K}\|_{L^\infty([a,b]^2,\mathbb{C}^{k\times k})}\}. \tag{2.313}$$

The following result gives a bound on the error between the Fredholm determinant, d_p, of an operator $\mathcal{K} \in \mathcal{J}_p$, for $p = 1$ or 2, and its numerical approximation, $d_{p,Q}$.

Theorem 2.5.3. *Let $\mathcal{K} \in \mathcal{J}_p(L^2([a,b],\mathbb{C}^k))$ be an operator with matrix-valued kernel $\boldsymbol{K} \in L^2([a,b]\times[a,b],\mathbb{C}^{k\times k})$. Suppose that $K_{ij} \in C^{0,1}([a,b]\times[a,b],\mathbb{C})$ is Lipschitz continuous for all $i,j \in \{1,\ldots,k\}$. Let Q denote the composite Simpson's quadrature rule with spacing Δx. Then*

$$|d_{p,Q}(z) - d_p(z)| \leq \frac{c_1}{2}\Delta x \boldsymbol{\Phi}(\beta|z|), \tag{2.314}$$

where c_1 is the constant in Theorem 2.5.2, $\beta = k(b-a)\|\boldsymbol{K}\|_{W^{1,\infty}}$, and

$$\boldsymbol{\Phi}(z) = \sum_{n=1}^{\infty} \frac{n^{(n+2)/2}}{n!} z^n. \tag{2.315}$$

Proof. As in Lemma A.4 of [26], we have

$$\left\| \left(\widetilde{K}_{\mathbf{j}}^{(n)}\right)^{(1)} \right\|_{L^\infty([a,b]^n)} \leq 2n^{(n+2)/2}\|\mathbf{K}\|_{W^{1,\infty}}^n \tag{2.316}$$

where $\widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x}) = \widetilde{K}_{\mathbf{j}}^{(n)}(\mathbf{x},\mathbf{x})$ is given by (2.243). By (2.284), we have that for $p = 1$ or 2,

$$|d_{p,Q}(z) - d_p(z)| \;\leq\; \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\mathbf{j}\in J_k^{(n)}} \left| Q^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)}) - \int_{[a,b]^n} \widetilde{K}_{\mathbf{j}}^{(n)}(x_1,\ldots,x_n)dx_1\ldots dx_n \right|.$$

Combining this with (2.312) and (2.289), we see that

$$\begin{aligned}
|d_{p,Q}(z)-d_p(z)| &\leq \sum_{n=1}^{\infty}\frac{|z|^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}\left|Q^{(n)}(\widetilde{K}_{\mathbf{j}}^{(n)})-\int_{[a,b]^n}\widetilde{K}_{\mathbf{j}}^{(n)}(x_1,\ldots,x_n)dx_1\ldots dx_n\right| \\
&\leq \frac{1}{4}\sum_{n=1}^{\infty}\frac{|z|^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}c_1(b-a)^n\Delta x\left\|\left(\widetilde{K}_{\mathbf{j}}^{(n)}\right)^{(1)}\right\|_{L^\infty([a,b]^n)} \\
&\leq c_1\frac{\Delta x}{4}\sum_{n=1}^{\infty}\frac{(|z|(b-a))^n}{n!}\sum_{\mathbf{j}\in J_k^{(n)}}\max_{\mathbf{j}\in J_k^{(n)}}\left\|\left(\widetilde{K}_{\mathbf{j}}^{(n)}\right)^{(1)}\right\|_{L^\infty([a,b]^n)} \\
&= c_1\frac{\Delta x}{4}\sum_{n=1}^{\infty}\frac{(|z|(b-a))^n}{n!}k^n\max_{\mathbf{j}\in J_k^{(n)}}\left\|\left(\widetilde{K}_{\mathbf{j}}^{(n)}\right)^{(1)}\right\|_{L^\infty([a,b]^n)} \\
&\leq c_1\frac{\Delta x}{4}\sum_{n=1}^{\infty}\frac{(|z|(b-a)k)^n}{n!}2n^{(n+2)/2}\|\mathbf{K}\|_{W^{1,\infty}}^n \\
&= \frac{c_1\Delta x}{2}\sum_{n=1}^{\infty}\frac{n^{(n+2)/2}}{n!}(|z|(b-a)k\|\mathbf{K}\|_{W^{1,\infty}})^n \\
&= \frac{c_1\Delta x}{2}\mathbf{\Phi}(|z|\beta). \qquad (2.317)
\end{aligned}$$

□

Note: Bornemann [26] shows that

$$\mathbf{\Phi}(z)\leq z\mathbf{\Psi}(z\sqrt{2}e), \qquad (2.318)$$

where

$$\mathbf{\Psi}(z)=1+\frac{\sqrt{\pi}}{2}ze^{z^2/4}\left[1+\operatorname{erf}\left(\frac{z}{2}\right)\right]. \qquad (2.319)$$

Therefore, the term $\mathbf{\Phi}(\beta|z|)$ in the quadrature error bound (2.314) is bounded above by a computable constant depending on $\|\mathbf{K}\|_{W^{1,\infty}}$.

CHAPTER 3

A CRITERION FOR A HILBERT-SCHMIDT OPERATOR TO BE TRACE CLASS

3.1 Introduction, Background, and Main Results

In this chapter we revisit a 120 year old problem from the birth of functional analysis on the trace and determinant of integral operators. The novelty of our contribution is that the operators we are concerned with are defined in terms of matrix-valued kernels rather than the scalar-valued kernels that are most commonly treated in the classical theory. Our interest in matrix-valued kernels comes from applications to the stability of pulse solutions of nonlinear wave equations such as the complex Ginzburg-Landau equation [22, 36, 37, 19]. Our goal is to establish a regularity criterion on a matrix-valued kernel which ensures that the corresponding integral operator is trace class and hence has a regular Fredholm determinant. Specifically, we will prove that if a matrix-valued kernel on a finite interval is Hölder continuous with Hölder exponent greater than a half, then the operator is trace class. We will show that an analogous result also holds for matrix-valued kernels on the real line, provided that an additional exponential decay assumption holds. While these results are not surprising, we have not been able to find statements or proofs of them in the literature. We will provide two proofs for matrix-valued kernels on a finite interval, both of which are based on classical proofs obtained for scalar-valued kernels. The first proof is based on a result of Weidmann from 1965 [38] that relies on ideas from Fourier analysis due to Hardy and Littlewood [39]. The second proof is inspired by a theorem in the book of Gohberg, Goldberg and Krupnik [30]. Their approach is based on a beautiful calculation of Fredholm in the seminal 1903 paper [25] where he first introduced the concept of the Fredholm determinant.

Our focus is on integral operators, $\mathcal{K}$, of the form

$$(\mathcal{K}\boldsymbol{\phi})(x) \;=\; \int_X \mathbf{K}(x,y)\boldsymbol{\phi}(y)\,dy, \tag{3.1}$$

where $\mathbf{K}$ is a matrix-valued kernel and X is either a finite interval, $X = [a, b]$, or the real line, $X = \mathbb{R}$. If $\mathbf{K} \in L^2(X \times X, \mathbb{C}^{k \times k})$ is a square-integrable complex matrix-valued function of x and y, then the corresponding operator $\mathcal{K}$ is a Hilbert-Schmidt operator on the Hilbert space, $L^2(X, \mathbb{C}^k)$, of square-integrable complex vector-valued functions, $\boldsymbol{\phi}$, on X. All such operators are compact. We recall that the space, $\mathcal{J}_2(\mathcal{H})$, of Hilbert-Schmidt operators on a Hilbert space, $\mathcal{H}$, is a Banach space in which the norm is given by the L^2-norm of the kernel. Since the composition of a bounded (resp. compact) operator and a Hilbert-Schmidt operator is Hilbert-Schmidt, the space $\mathcal{J}_2(\mathcal{H})$ is an ideal in the set of bounded (resp. compact) operators.

Trace class operators are compact operators on a Hilbert space for which a notion of trace can be defined.[1] The theory of trace class operators was developed by Schatten and von Neumann in the 1940's [40]. They defined an operator $\mathcal{K}$ on $\mathcal{H}$ to be trace class if it is the composition of two Hilbert-Schmidt operators. Because $J_2(\mathcal{H})$ is an ideal, every trace class operator is Hilbert-Schmidt. They defined the trace of $\mathcal{K}$ by

$$\mathrm{Tr}(\mathcal{K}) = \sum_{\ell} \langle \phi_\ell, \mathcal{K}\phi_\ell \rangle, \tag{3.2}$$

where $\{\phi_\ell\}$ is any orthonormal basis for $\mathcal{H}$. Equivalently, the trace of $\mathcal{K}$ is the sum of the singular values, μ_ℓ, of $\mathcal{K}$, which are the nonnegative real numbers so that the ℓ-th eigenvalue of the Hermitian symmetric operator $\mathcal{K}^*\mathcal{K}$ is μ_ℓ^2. In 1959, Lidskii proved that the trace of $\mathcal{K}$ is the sum of its eigenvalues, λ_ℓ, counted with algebraic multiplicity [41],

$$\mathrm{Tr}(\mathcal{K}) = \sum_{\ell} \lambda_\ell. \tag{3.3}$$

Following Simon [24], we define a compact operator, $\mathcal{K}$, on $\mathcal{H}$ to belong to the p-th Schatten class, $J_p(\mathcal{H})$, if the ℓ_p-norm of the sequence, $\{\mu_\ell\}$, of singular values of $\mathcal{K}$ is finite,

[1] For a detailed history of the subject and a comprehensive literature review, we refer the reader to the books of Barry Simon [24] and Gohberg, Goldberg and Krupnik [30], as well as to the recent influential paper of Bornemann [26] on the numerical evaluation of Fredholm determinants.

i.e, if

$$\|\mathcal{K}\|_{J_p(\mathcal{H})} := \sum_\ell |\mu_\ell|^p < \infty. \tag{3.4}$$

The cases $p = 1$ and $p = 2$ are the spaces of trace class and Hilbert-Schmidt operators, respectively.

A major reason for the interest in trace class operators is that $J_1(\mathcal{H})$ is a space of operators for which the regular Fredholm determinant is defined. Following Simon [24] and Grothendieck [42], if $\mathcal{K}$ is trace class on $\mathcal{H}$, then for each k the k-th wedge product, $\Lambda^k\mathcal{K}$, is trace class on $\Lambda^k\mathcal{H}$ and the infinite series

$$\det{}_1(\mathcal{I} + z\mathcal{K}) \;:=\; \sum_{n=0}^{\infty} z^n \operatorname{Tr}(\Lambda^n\mathcal{K}) \tag{3.5}$$

defines an entire function of $z \in \mathbb{C}$. As in the finite rank case (see [24] for a proof),

$$\det{}_1(\mathcal{I} + z\mathcal{K}) \;=\; \prod_{\ell=1}^{\infty}(1 + z\lambda_\ell). \tag{3.6}$$

If the operator $\mathcal{K}$ is Hilbert-Schmidt but not trace class, it is still possible to define a Fredholm determinant for $\mathcal{K}$. To do so, we first observe that the operator $R_2(\mathcal{K}) := (1 + \mathcal{K})e^{-\mathcal{K}} - 1$ is trace class [24], since it is of the form $R_2(\mathcal{K}) = \mathcal{K}^2 h(\mathcal{K})$ for some entire function, h, and the square of a Hilbert-Schmidt operator is trace class. The 2-modified Fredholm determinant is then defined by

$$\det{}_2(\mathcal{I} + z\mathcal{K}) \;:=\; \det{}_1(1 + R_2(z\mathcal{K})) \;=\; \det{}_1\left((1 + z\mathcal{K})e^{-z\mathcal{K}}\right), \tag{3.7}$$

which is once again an entire function of z. In this case, the infinite product

$$\det{}_2(\mathcal{I} + z\mathcal{K}) \;=\; \prod_{\ell=1}^{\infty}\left[(1 + z\lambda_\ell)e^{-z\lambda_\ell}\right] \tag{3.8}$$

converges. Furthermore, if $\mathcal{K}$ is trace class, then both Fredholm determinants are defined,

$$\det{}_2(\mathcal{I} + z\mathcal{K}) \;=\; \det{}_1(\mathcal{I} + z\mathcal{K})\, e^{-\operatorname{Tr}(\mathcal{K})}, \tag{3.9}$$

and the zeros of $\det_2(\mathcal{I}+z\mathcal{K})$ and $\det_1(\mathcal{I}+z\mathcal{K})$ coincide.

Fredholm determinants were introduced by Fredholm [25] to characterize the solvability of integral equations of the second kind, $(\mathcal{I}+z\mathcal{K})\boldsymbol{\phi}=\boldsymbol{\psi}$. For applications of Fredholm determinants in mathematical physics, see Simon [24] and Bornemann [26]. Our interest in them stems from the fact that the set of eigenvalues of the linearization of the complex Ginzburg-Landau equation about a stationary (soliton) solution is given by the set of zeros of a Fredholm determinant of a Birman-Schwinger operator that is defined in terms of a matrix-valued Green's kernel on the real line [20].

Since trace class operators are Hilbert-Schmidt, every trace class operator, $\mathcal{K}$, on $L^2(X,\mathbb{C}^k)$ has a kernel, $\mathbf{K}\in L^2(X\times X,\mathbb{C}^{k\times k})$, as in (3.1). However, there is no simple necessary and sufficient condition on a kernel $\mathbf{K}$ that guarantees that $\mathcal{K}$ is trace class. In the scalar case, there are however regularity conditions on $\mathbf{K}$ that imply that $\mathcal{K}$ is trace class.

The first major result in this direction is Mercer's Theorem [43] which, in the case of a matrix valued kernels, states that if $\mathbf{P}$ is a continuous, non-negative definite Hermitian kernel on a finite interval, $[a,b]$, then the corresponding operator $\mathcal{P}$ is trace class. In a nutshell the proof is that there is an orthonormal set, $\{\boldsymbol{\phi}_j\}$, of continuous eigenfunctions in $L^2([a,b],\mathbb{C}^k)$ and non-negative eigenvalues, λ_ℓ , so that

$$\mathbf{P}(x,y) \;=\; \sum_\ell \lambda_\ell \boldsymbol{\phi}_\ell(x)\boldsymbol{\phi}_\ell^*(y), \tag{3.10}$$

where the series converges absolutely and uniformly. Consequently, we can exchange integrals and sums to conclude that (because $\mathbf{P}$ is continuous on the diagonal)

$$\infty > \int_a^b \operatorname{Tr}(\mathbf{P}(x,x))\,dx = \sum_\ell \lambda_\ell = \sum_\ell |\mu_\ell|, \tag{3.11}$$

where the last equality follows from the fact that $\mathcal{P}\geq 0$.

It is not possible to drop the definiteness assumption in Mercer's Theorem since Carlemann [44] constructed a C^0-function, k, whose Fourier coefficients are in ℓ_2 but not in ℓ_1.

Consequently, the operator with continuous kernel $K(x,y) = k(x-y)$ is not trace class. Subsequently, for each Hölder exponent, $\gamma \leq 1/2$, Bernstein [45] constructed a function in the Hölder space, $C^{0,\gamma}$, with the same property. Therefore, to guarantee that an operator is trace class, the kernel must be at least $C^{0,1/2}$. If a scalar kernel is C^1 then a simple integration by parts argument shows that the corresponding operator is trace class [26, 46]. However, the C^1 condition can be overly restrictive. For example, for the Birman-Schwinger integral operators we are interested in the kernel, $\mathbf{K} = \mathbf{K}(x,y)$, is continuous, but not differentiable, across the diagonal, $y = x$. Nevertheless, under some reasonable assumptions that are easy to check, we can show that $\mathbf{K} \in C^{0,1}$ is Lipschitz-continuous.

We are now in a position to state our main theorems. First, in the case of operators on a finite interval we have the following result.

Theorem 3.1.1. *Let $\mathcal{K} \in \mathcal{J}_2(L^2([a,b],\mathbb{C}^k))$ be a Hilbert-Schmidt operator on a finite interval, $[a,b]$, that is defined in terms of a matrix-valued kernel $\boldsymbol{K} \in L^2([a,b]\times[a,b],\mathbb{C}^{k\times k})$ by (3.1). Suppose that $\mathbf{K}$ is continuous on $[a,b]\times[a,b]$ and satisfies the Hölder-continuity condition*

$$|K_{pq}(x_1,y_1) - K_{pq}(x_2,y_2)| \;\leq\; C\|(x_1,y_1) \;-\; (x_2,y_2)\|^{\gamma}, \tag{3.12}$$

for all $p,q \in \{1,\cdots,k\}$, for some constants $C > 0$ and $\frac{1}{2} < \gamma \leq 1$. Then, $\mathcal{K} \in \mathcal{J}_1(L^2([a,b],\mathbb{C}^k))$ is trace class.

Using a change of variables from a finite interval to the entire real line, we can transform this result to obtain an analogous result for kernels on the real line that decay exponentially. For simplicity, for this result we assume that the kernel is Lipschitz continuous rather than being Hölder continuous. The reason for making this assumption is that Lipschitz continuous functions are differentiable almost everywhere, whereas functions that are merely Hölder continuous may not be.

Theorem 3.1.2. *Let $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^k))$ be a Hilbert-Schmidt operator on the real line that is defined in terms of a matrix-valued kernel $\boldsymbol{K} \in L^2(\mathbb{R} \times \mathbb{R}, \mathbb{C}^{k \times k})$. Suppose that $\mathbf{K}$ satisfies the Lipschitz continuity condition*

$$|K_{pq}(x_1, y_1) - K_{pq}(x_2, y_2)| \; \leq \; C\|(x_1, y_1) \; - \; (x_2, y_2)\|, \tag{3.13}$$

for all $p, q \in \{1, \cdots, k\}$, for some constant $C > 0$. Furthermore, suppose that $\boldsymbol{K}$ and both of its first partial derivatives decay exponentially, such that for almost all $x, y \in \mathbb{R}$

$$\max\{\|\boldsymbol{K}(x, y)\|, \|\partial_x \boldsymbol{K}(x, y)\|, \|\partial_y \boldsymbol{K}(x, y)\|\} \leq Ce^{-\alpha|x-y|}, \tag{3.14}$$

for some $C, \alpha > 0$. Then, $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R}, \mathbb{C}^k))$ is trace class.

The proof of Theorem 3.1.2 is given in Section 3.4 below. We have two proofs of Theorem 3.1.1. In the next two sections, we will outline the major ideas of these two proofs. The technical details we will provided in a forthcoming paper [47].

3.2 Outline of First Proof of Theorem 3.1.1

Here we outline how to extend Weidmann's proof [38] to matrix-valued kernels. The basic idea is to show that if the kernel, $\mathbf{K}$ for $\mathcal{K}$ is $C^{0,\gamma}$ with $\gamma > 1/2$, then the non-negative definite Hermitian operator, $\mathcal{P} = (\mathcal{K}\mathcal{K}^*)^{1/2}$ has a kernel that is continuous. Therefore, by Mercer's Theorem, $\mathcal{P}$ is trace class. Consequently, $\mathcal{K}$ is also trace class since (by definition) it has has the same singular values as $\mathcal{P}$. Since Weidmann's paper, which is in German, is not so easy to follow, we provide some additional details.

We first apply the spectral theorem for compact Hermitian operators to obtain the eigenfunction expansion

$$(\mathcal{K}^*\mathcal{K})(\boldsymbol{\psi}) \; = \; \sum_{\ell=1}^{\infty} \mu_\ell^2 \langle \boldsymbol{\phi}_\ell, \boldsymbol{\psi} \rangle \boldsymbol{\phi}_\ell, \tag{3.15}$$

which converges in $L^2(\mathbb{R}, \mathbb{C}^k)$, where $\{\boldsymbol{\phi}_\ell\}$ is an orthonormal set of continuous eigenfunctions of $\mathcal{K}^*\mathcal{K}$ with eigenvalues, $\{\mu_\ell^2\}$. Similarly,

$$(\mathcal{K}\mathcal{K}^*)(\boldsymbol{\psi}) \;=\; \sum_{\ell=1}^{\infty} \mu_\ell^2 \langle \boldsymbol{\psi}_\ell, \boldsymbol{\psi} \rangle \boldsymbol{\psi}_\ell, \tag{3.16}$$

where the functions, $\boldsymbol{\psi}_\ell := \mu_\ell^{-1}\mathcal{K}\boldsymbol{\phi}_\ell$, form an orthonormal set of continuous eigenfunctions for $\mathcal{K}\mathcal{K}^*$ with the same eigenvalues. The kernel for the operator $\mathcal{L} = \mathcal{K}\mathcal{K}^*$ is given by

$$\mathbf{L}(x, y) \;=\; \int_a^b \mathbf{K}(x, z)\mathbf{K}^*(z, y)\, dz, \tag{3.17}$$

where $\mathbf{K}^*(x, y) = [\overline{\mathbf{K}(y, x)}]^T$. Therefore, since $\mathbf{K}$ is continuous, the kernel $\mathbf{L}$ is continuous, non-negative definite Hermitian. So by Mercer's Theorem

$$\mathbf{L}(x, y) \;=\; \sum_{\ell=1}^{\infty} \mu_\ell^2 \boldsymbol{\psi}_\ell(x)\boldsymbol{\psi}_\ell^*(y), \tag{3.18}$$

converges uniformly and absolutely. Here, $\boldsymbol{\psi}_\ell(x)$ is a column vector and $\boldsymbol{\psi}_\ell^*(y)$ is a row vector. In particular, since $\mathcal{L}$ is trace class,

$$\sum_{\ell=1}^{\infty} \mu_\ell^2 \;<\; \infty. \tag{3.19}$$

Moreover,

$$\operatorname{Tr} \mathbf{L}(x, x) \;=\; \sum_{\ell=1}^{\infty} \mu_\ell^2 \|\boldsymbol{\psi}_\ell(x)\|_{\mathbb{C}^k}^2 \;<\; \infty. \tag{3.20}$$

Next, we observe that by [43, Theorem 14.3], the Hilbert-Schmidt operator, $\mathcal{K} \in J_2(L^2([a, b], \mathbb{C}^k))$, has the eigenfunction expansion

$$\mathcal{K}(\boldsymbol{\psi}) \;=\; \sum_{\ell=1}^{\infty} \mu_\ell \langle \boldsymbol{\psi}, \boldsymbol{\phi}_\ell \rangle \boldsymbol{\psi}_\ell \qquad \text{in } L^2([a, b], \mathbb{C}^k). \tag{3.21}$$

Since $\mathcal{K}$ is Hilbert-Schmidt, this implies that $\mathcal{K}$ has the matrix-valued kernel

$$\mathbf{K}(x, y) \;=\; \sum_{\ell=1}^{\infty} \mu_\ell \boldsymbol{\psi}_\ell(x)\boldsymbol{\phi}_\ell^*(y), \tag{3.22}$$

where the series converges in $L^2([a,b]\times[a,b],\mathbb{C}^{k\times k})$. More importantly for our purposes, by (3.20), for each $x\in[a,b]$ the series in (3.22) converges as a function of y in $L^2([a,b],\mathbb{C}^k)$.

The kernel for the operator $\mathcal{P}:=\mathcal{L}^{1/2}$ is given by

$$\mathbf{P}(x,y) \;=\; \sum_{\ell=1}^{\infty}\mu_\ell\boldsymbol{\psi}_\ell(x)\boldsymbol{\psi}_\ell^*(y), \tag{3.23}$$

which converges in the same sense as does (3.22). Note that we do not have any control of the uniform (or even pointwise) convergence of the series (3.23). Consequently, even though each term in the series is continuous, we cannot conclude that the kernel, $\mathbf{P}$, is continuous. However, in [38] Weidmann proved that if the kernel, $\mathbf{P}$, satisfies a certain integrated Hölder continuity condition then there is a continuous kernel, $\mathbf{P}_0$, so that $\mathbf{P}(x,y)=\mathbf{P}_0(x,y)$ for almost all x,y. In the special case we need, Weidmann's theorem is as follows.

Theorem 3.2.1. *Suppose that $P\in L^2([a,b]\times[a,b],\mathbb{C})$ is a scalar-valued kernel for which there is a $\gamma\in(1/2,1]$ so that*

$$\int_a^b |P(x,y)-P(x',y)|^2\,dy \;\le\; C|x-x'|^{2\gamma} \tag{3.24}$$

$$\int_a^b |P(x,y)-P(x,y')|^2\,dx \;\le\; C|y-y'|^{2\gamma} \tag{3.25}$$

for all $x,x',y,y'\in[a,b]$. Then there is a kernel $P_0\in C^{0,\gamma-1/2}([a,b]\times[a,b],\mathbb{C})$ so that $P(x,y)=P_0(x,y)$ for almost all x,y. In particular, the kernel P_0 is continuous.

Remark. *To convert the integrated Hölder conditions* (3.24) *and* (3.25) *into a pointwise condition, Weidmann averages the kernel, P, over a small rectangle of side length, d, to obtain*

$$P_d(x,y) \;=\; \frac{1}{d^2}\iint_{[-d/2,d/2]^2} P(x+\xi,y+\eta)\,d\xi\,d\eta. \tag{3.26}$$

He then uses an argument that applies Hölder's inequality to the inner integrals $\int_{[-d/2,d/2]}|P_d(x,y)-P_d(x',y)|\,dy$ and $\int_{[-d/2,d/2]}|P_d(x,y)-P_d(x,y')|\,dx$ to conclude that there is a constant, C, independent of d, so that $P_d\in C^{0,\gamma-1/2}([a,b]\times[a,b],\mathbb{C})$. Applying the

Arzela-Ascoli Theorem, he concludes that there is a sequence $d_n \to 0$ *so that* $P_{d_n} \to P_0$ *with* $P_0 \in C^{0,\gamma-1/2}([a,b]\times[a,b],\mathbb{C})$.

To show that Weidmann's theorem applies we argue as follows. First, we observe that, by (3.22) and (3.23), for each $x \in [a,b]$, and each pair of matrix indices, (p,q), the functions $y \mapsto \mathbf{K}_{pq}(x,y)$ and $y \mapsto \mathbf{P}_{pq}(x,y)$ have the same coefficients, $\mu_\ell \boldsymbol{\psi}_{\ell,p}(x)$, but are expressed in two different orthonormal sets, namely $\{\boldsymbol{\phi}_{\ell,q}\}$ and $\{\boldsymbol{\psi}_{\ell,q}\}$, where $\boldsymbol{\psi}_{\ell,p}(x)$ denotes the p-th entry of the vector $\boldsymbol{\psi}_\ell(x)$. Consequently, if $\|\mathbf{M}\|_F^2 := \sum_{p,q=1}^{k} \mathbf{M}_{pq}^2$ denotes the Frobenius norm of a matrix, $\mathbf{M}$, then

$$\begin{aligned}\int_a^b \|\mathbf{P}(x,y)-\mathbf{P}(x',y)\|_F^2\,dy &= \sum_{\ell=1}^{\infty} \mu_\ell^2 \|\boldsymbol{\psi}_\ell(x)-\boldsymbol{\psi}_\ell(x')\|_{\mathbb{C}^k}^2 \\ &= \int_a^b \|\mathbf{K}(x,y)-\mathbf{K}(x',y)\|_F^2\,dy. \end{aligned} \tag{3.27}$$

Therefore, by integrating the Hölder continuity condition, (3.12), for $\mathbf{K}$, in Theorem 3.1.1, and applying (3.27), we find that (3.24) holds for $\mathbf{P}_{pq}$. A similar argument shows that (3.25) also holds. Therefore, the operator $\mathcal{P}$ has a continuous kernel, and so by Mercer's Theorem is trace class.

3.3 Outline of Second Proof of Theorem 3.1.1

The main idea for the second proof is contained in Fredholm's 1903 paper [25]. Of course at that point, Fredholm did not quite have the concept of a trace class operator. Rather he proved that if a scalar-valued kernel, $K : [a,b]\times[a,b] \to \mathbb{C}$, for an integral operator, $\mathcal{K}$, satisfies the Hölder continuity condition

$$|K(x,y_1) - K(x,y_2)| \le C|y_1 - y_2|^\gamma \tag{3.28}$$

for a Hölder exponent, $\gamma \in (0,1]$, and if

$$b_n(\mathcal{K}) := \frac{1}{n!} \int\limits_{[a,b]^n} \det[K(x_\alpha, x_\beta)]_{\alpha,\beta=1}^n \, dx_1 \cdots dx_n, \tag{3.29}$$

then the infinite series,

$$D_{\mathcal{K}}(z) \;:=\; \sum_{n=0}^{\infty} b_n(\mathcal{K}) z^n, \tag{3.30}$$

converges uniformly and absolutely to an entire function of the complex parameter, z. Fredholm then uses (3.30) as the definition of his determinant. In modern parlance, we note that if the operator is already known to be trace class, then the regular Fredholm determinant of $\mathcal{K}$ is given by

$$\det(\mathcal{I} + z\mathcal{K}) \;=\; D_{\mathcal{K}}(z). \tag{3.31}$$

To prove that the series (3.30) converges, Fredholm used an ingenious combination of estimates to show that there is a constant, C_1 so that

$$|b_n(\mathcal{K})| \;\leq\; \frac{C_1^n}{n!}\, n^{-\gamma+1/2}. \tag{3.32}$$

We note that this estimate only holds for operators defined on a finite interval, not on the entire real line.

In their 2000 text *Traces and Determinants of Linear Operators*, Gohberg, Goldberg, and Krupnik [30] use this estimate to prove that if the operator $\mathcal{K}$ is Hermitian symmetric and if the Hölder exponent satisfies $\gamma > 1/2$, then $\mathcal{K}$ is trace class. Their proof is based on two main ideas. The first idea is to show that $D_{\mathcal{K}}(z)$ is the limit in an appropriate sense of a sequence of finite dimensional determinants, $\det(I + zK_m)$, for $m \in \mathbb{N}$. Consequently, the set of eigenvalues, $\{\lambda_j\}$, of the Hermitian symmetric operator $\mathcal{K}$ coincides with the set $\{-1/z_j\}$, where $\{z_j\}$ is the set of zeros of the entire function $D_{\mathcal{K}}(z)$. The second idea is to use a result from the theory of the distribution of the zeros of entire functions [48] to show that the series

$$\sum_j |\lambda_j| \;=\; \sum_j \frac{1}{|z_j|} \tag{3.33}$$

converges if the order of growth,

$$\rho_D \;:=\; \limsup_{n\to\infty} \frac{n \log n}{\log \frac{1}{|b_n|}}, \tag{3.34}$$

of the entire function $D_{\mathcal{K}}(z)$ satisfies $\rho_D < 1$. By (3.32), this inequality holds provided that $\gamma > 1/2$. Finally we observe that if $\mathcal{K}$ is Hermitian then $|\lambda_j| = \mu_j$, and so the convergence of (3.33) implies that $\mathcal{K}$ is trace class.

To extend this proof to matrix-valued kernels without making the additional assumption that the operator is Hermitian symmetric, we first note that if Theorem 3.1.1 holds for Hermitian operators, then it holds for operators that are not assumed to have any symmetry properties. To see this, we begin by recalling that the Hermitian inner product on $L^2([a,b],\mathbb{C}^k)$ is defined by

$$\langle \boldsymbol{\phi}, \boldsymbol{\psi} \rangle_{L^2([a,b],\mathbb{C}^k)} := \int_a^b \boldsymbol{\phi}^*(x)\boldsymbol{\psi}(x)\,dx, \tag{3.35}$$

where $\boldsymbol{\phi}^* = \overline{\boldsymbol{\phi}}^T$ is conjugate transpose. Consequently, the Hermitian adjoint of the operator, $\mathcal{K}$, is the operator, $\mathcal{K}^*$, with kernel $\mathbf{K}^*$ defined by $\mathbf{K}^*(x,y) := \overline{[\mathbf{K}(y,x)]}^T$.

Let

$$\mathbf{H} := \frac{\mathbf{K}+\mathbf{K}^*}{2} \qquad \text{and} \qquad \mathbf{S} := \frac{\mathbf{K}-\mathbf{K}^*}{2} \tag{3.36}$$

be the Hermitian and skew-Hermitian parts of $\mathbf{K}$. Since the kernel $\widetilde{\mathbf{S}} = i\mathbf{S}$ is Hermitian, we see that $\mathbf{K} = \mathbf{H} - i\widetilde{\mathbf{S}}$ is a linear combination of Hermitian kernels, each of which is continuous and satisfies the Hölder-continuity condition (3.12). Since the space of trace class operators is a vector space, we conclude that if the result is true for Hermitian operators, then it is true in general.

One of the challenges in the approach of Gohberg, Goldberg, and Krupnik is that they had to develop a theory of determinants of compact operators that is parallel to but distinct from the theory of regular and 2-modified Fredholm determinants of trace class and Hilbert-Schmidt operators. They use their theory to show that $D_{\mathcal{K}}(z)$ is the limit of a sequence of finite dimensional determinants and that $\lambda_j = -1/z_j$.

Rather than relying on this theory, since we already know that $\mathcal{K}$ is Hilbert-Schmidt, we can replace $D_{\mathcal{K}}(z)$ in (3.30) with the 2-modified Fredholm determinant, which in the case of a matrix-valued kernel, is the entire function

$$\det_2(\mathcal{I} + z\mathcal{K}) \;:=\; \sum_{n=0}^{\infty} \sum_{\mathbf{j}\in J_k^{(n)}} b_{n,\mathbf{j}}(\mathcal{K})\, z^n, \tag{3.37}$$

where

$$b_{n,\mathbf{j}}(\mathcal{K}) \;=\; \frac{1}{n!} \int\limits_{[a,b]^n} \det\left[K_{j_\alpha j_\beta}(x_\alpha, x_\beta)(1-\delta_{\alpha\beta})\right]_{\alpha,\beta=1}^{n}, dx_1 \cdots dx_n. \tag{3.38}$$

Using (3.38), we can derive a version of Fredholm's estimate (3.32), the details of which are in [47]. Finally, we use (3.8) to complete the proof.

3.4 Proof of Theorem 3.1.2

To generalize Theorem 3.1.1 to the case of a Hilbert-Schmidt integral operator, $\mathcal{K}$, with Lipschitz-continuous matrix-valued kernel on $\mathbb{R}$, we use a scaling mapping, $\phi : (-1,1) \to \mathbb{R}$, to transform $\mathcal{K}$ to an operator, $\widetilde{\mathcal{K}}$, on $(-1,1)$ that is given by $\widetilde{\mathcal{K}} = \mathcal{U}\mathcal{K}\mathcal{U}^{-1}$, where $\mathcal{U} : L^2(\mathbb{R}, \mathbb{C}^k) \to L^2((-1,1), \mathbb{C}^k)$ is an isometry defined in terms of ϕ. We will show that if the kernel $\mathbf{K}$ for $\mathcal{K}$ is Lipschitz-continuous, then so is the transformed kernel, $\widetilde{\mathbf{K}}$ for $\widetilde{\mathcal{K}}$. Therefore, by Theorem 3.1.1, $\widetilde{\mathbf{K}}$ is trace class. Finally, since the operators $\mathcal{K}$ and $\widetilde{\mathbf{K}}$ are related by a similarity transform, they have the same singular values, which implies that $\mathcal{K}$ is also trace class.

To define the scaling transformation $\phi : (-1,1) \to \mathbb{R}$, for reasons that will become apparent later, we fix $\delta \in (0, \alpha/3)$ (here α is the exponential decay constant in (3.14)) and set

$$x = \phi(y) := \frac{1}{2\delta} \log \frac{1+y}{1-y}. \tag{3.39}$$

Then

$$\phi'(y) = \frac{1}{\delta} \frac{1}{1-y^2} > 0, \tag{3.40}$$

and the inverse map, $\phi^{-1} : \mathbb{R} \to (-1,1)$, is given by

$$y = \phi^{-1}(x) := \tanh(\delta x) = \frac{e^{\delta x} - e^{-\delta x}}{e^{\delta x} + e^{-\delta x}}. \tag{3.41}$$

The operator $\mathcal{U} : L^2(\mathbb{R}, \mathbb{C}^k) \to L^2((-1,1), \mathbb{C}^k)$ is defined by

$$(\mathcal{U}\mathbf{f})(y) = (\phi'(y))^{1/2}\mathbf{f}(\phi(y)), \quad \mathbf{f} \in L^2(\mathbb{R}, \mathbb{C}^k). \tag{3.42}$$

and $\mathcal{U}^{-1} : L^2((-1,1), \mathbb{C}^k) \to L^2(\mathbb{R}, \mathbb{C}^k)$ is given by

$$(\mathcal{U}^{-1}\mathbf{g})(x) = ((\phi^{-1})'(x))^{1/2}\mathbf{g}(\phi^{-1}(x)), \quad \mathbf{g} \in L^2((-1,1), \mathbb{C}^k). \tag{3.43}$$

These operators are isometries, since by the change of variables theorem,

$$\|\mathcal{U}\mathbf{f}\|^2_{L^2((-1,1),\mathbb{C}^k)} = \int_{-1}^{1} \|\mathbf{f}(\phi(y))\|^2\phi'(y)dy = \int_{-\infty}^{\infty} \|\mathbf{f}(x)\|^2 dx = \|\mathbf{f}\|^2_{L^2(\mathbb{R},\mathbb{C}^k)}, \tag{3.44}$$

and similarly for $\mathcal{U}^{-1}$.

Next we claim that the kernel for the operator $\widetilde{\mathcal{K}} = U\mathcal{K}U^{-1}$ on $L^2((-1,1), \mathbb{C}^k)$ is given by

$$\widetilde{\mathbf{K}}(y, y') = (\phi'(y))^{1/2}\mathbf{K}(\phi(y), \phi(y'))(\phi'(y'))^{1/2},\ y, y' \in (-1,1). \tag{3.45}$$

We verify (3.45) by applying the chain rule and the change of variables $x' = \phi(y')$, to obtain

$$\begin{aligned}(\widetilde{\mathcal{K}}\mathbf{g})(y) &= (\phi'(y))^{1/2} \int_{-\infty}^{\infty} \mathbf{K}(\phi(y), x')((\phi^{-1})'(x'))^{1/2}\mathbf{g}(\phi^{-1}(x'))dx' \\ &= (\phi'(y))^{1/2} \int_{-1}^{1} \mathbf{K}(\phi(y), \phi(y'))(\phi'(y'))^{1/2}\mathbf{g}(y')dy'.\end{aligned} \tag{3.46}$$

Although $\phi'(y)$ has singularities at $y = \pm 1$, $\widetilde{\mathbf{K}}$ is continuous on $[-1,1] \times [-1,1]$, since

$$\lim_{y \to \pm 1} \widetilde{\mathbf{K}}(y, y') = 0 = \lim_{y' \to \pm 1} \widetilde{\mathbf{K}}(y, y'). \tag{3.47}$$

To prove (3.47), we first observe that since $\alpha > \delta$,

$$e^{-\alpha|\phi(y)|} = \exp\left(\frac{-\alpha}{2\delta}\left|\log\frac{1+y}{1-y}\right|\right) = \begin{cases} \frac{1-y}{1+y}^{\alpha/(2\delta)},\ y \in [0,1), \\ \frac{1+y}{1-y}^{\alpha/(2\delta)},\ y \in (-1,0]. \end{cases} \tag{3.48}$$

Let us define

$$F_{\pm}(y) := \frac{(1 \mp y)^{\alpha/2\delta}}{(1 \pm y)^{\alpha/2\delta}(1-y^2)^{1/2}}. \tag{3.49}$$

Then, for $y \geq 0$, for example,

$$\lim_{y \to 1} \|(\phi'(y))^{1/2}\mathbf{K}(\phi(y), \phi(y'))(\phi'(y'))^{1/2}\| = \frac{C}{\delta} \lim_{y \to 1} F_+(y) F_\pm(y'). \tag{3.50}$$

Furthermore, since $\delta < \alpha/2$,

$$\lim_{y \to 1} F_+(y) = \lim_{y \to 1} \frac{(1-y)^{\alpha/(2\delta)}}{(1-y^2)^{1/2}(1+y)^{\alpha/(2\delta)}} = 0, \tag{3.51}$$

and

$$\lim_{y \to -1} F_-(y) = \lim_{y \to -1} \frac{(1+y)^{\alpha/(2\delta)}}{(1-y^2)^{1/2}(1-y)^{\alpha/(2\delta)}} = 0. \tag{3.52}$$

Therefore, for $y = \pm 1$ and $y' \in [-1, 1]$,

$$\lim_{y \to \pm 1} \|(\phi'(y))^{1/2}\mathbf{K}(\phi(y), \phi(y'))(\phi'(y'))^{1/2}\| = 0, \tag{3.53}$$

and the same will hold for $y' = \pm 1$, when $y \in [-1, 1]$. A similar argument holds for $\nabla \widetilde{\mathbf{K}}$, since

$$\begin{aligned} \partial_y \widetilde{\mathbf{K}}(y, y') &= (\phi'(y))^{1/2} \partial_y \mathbf{K}(\phi(y), \phi(y'))(\phi'(y'))^{1/2} \\ &\quad + [(\phi'(y))^{1/2}]' \mathbf{K}(\phi(y), \phi(y'))(\phi'(y'))^{1/2}. \end{aligned} \tag{3.54}$$

Since, by assumption, both $\partial_x \mathbf{K}$ and $\partial_y \mathbf{K}$ share the same exponential decay as $\mathbf{K}$, the first term in (3.54) converges to 0 as $y \to \pm 1$ or $y' \to \pm 1$ just as in (3.53) above. For the second term, we observe that since $\delta < \alpha/3$,

$$\lim_{y \to 1} \|[(\phi'(y))^{1/2}]' \mathbf{K}(\phi(y), \phi(y'))\| \leq \frac{C}{\sqrt{\delta}} \lim_{y \to 1} \frac{y}{(1-y^2)^{3/2}} \frac{(1-y)^{\alpha/(2\delta)}}{(1+y)^{\alpha/(2\delta)})} \tag{3.55}$$

$$= \frac{C}{\sqrt{\delta}} \lim_{y \to 1} \frac{y(1-y)^{\frac{1}{2}(\frac{\alpha}{\delta} - 3)}}{(1+y)^{\frac{1}{2}(\frac{\alpha}{\delta} + 3)}} \tag{3.56}$$

$$= 0. \tag{3.57}$$

To summarize, the scaled kernel, $\widetilde{\mathbf{K}}$, is differentiable almost everywhere with bounded derivative, and hence is Lipschitz. The result now follows as explained above.

CHAPTER 4

STATIONARY SOLUTIONS OF THE CQ-CGLE

In this chapter, we apply the results from Chapters 2 and 3 to the specific case of the cubic-quintic complex Ginzburg-Landau equation (CQ-CGLE) and its associated integral operators $\mathcal{K} \in \mathcal{J}_p(\mathbb{R}, \mathbb{C}^4)$, for $p = 1, 2$.

First, we linearize the CQ-CGLE about a stationary solution,Ψ, to define a second-order linear operator $\mathcal{L}$, whose spectrum characterizes the linear stability of the stationary pulse. We additionally define the asymptotic operator, $\mathcal{L}_\infty$, associated with $\mathcal{L}$. Since $\mathcal{L}$ is a relatively compact perturbation of $\mathcal{L}_\infty$, it shares certain spectral qualities with $\mathcal{L}_\infty$, whose spectrum is easier to compute. In Section 4.1, we define the unperturbed and perturbed first-order systems, which are of the form

$$\partial_x \mathbf{Y} = \mathbf{A}_\infty(\lambda)\mathbf{Y} \tag{4.1}$$

$$\partial_x \mathbf{Y} = (\mathbf{A}_\infty + \mathbf{R}(x))\mathbf{Y}, \tag{4.2}$$

and which are associated with the eigenvalue problems $\mathcal{L}\mathbf{\Psi} = \lambda\mathbf{\Psi}$ and $\mathcal{L}_\infty\mathbf{\Psi} = \lambda\mathbf{\Psi}$, respectively. Here, $\mathbf{Y} = \mathbf{Y}(x) \in \mathbb{C}^4$, and $\mathbf{A}_\infty(\lambda), \mathbf{R}(x) \in \mathbb{C}^{4\times4}$.

In Section 4.2, we diagonalize the first-order unperturbed problem and calculate the eigenvalues and eigenvectors of the asymptotic matrix $\mathbf{A}_\infty(\lambda)$. In Section 4.3, we define and compute the Bohl and Lyapunov exponents of the spectral projection $\mathbf{Q}(\lambda)$ onto the stable subspace of $\mathbf{A}_\infty(\lambda)$, which describe the exponential decay of the fundamental solutions of the unperturbed problem, and are used to guarantee existence and uniqueness of Jost solutions to the perturbed problem on the real line. The Jost solutions play a major role in the theory and computation of the Evans function [20].

In Section 4.4, to define the integral operator $\mathcal{K}(\lambda)$ associated with the pulse Ψ, we apply the well-known Birman-Schwinger principle. To form $\mathcal{K}$, we decompose the perturbation operator, $\mathbf{R}$ into two parts, $\mathbf{R} = \mathbf{R}_\ell \mathbf{R}_r$. Then we discuss conditions on $\mathcal{K}(\lambda)$ under which λ is in the point spectrum (is an eigenvalue) of $\mathcal{L}$.

Under reasonable decay conditions on the stationary pulse Ψ, we can guarantee that our integral operator $\mathcal{K}$ is Hilbert-Schmidt. In Section 4.5, we define the matrix-valued integral kernel, $\mathbf{K}$, associated with our integral operator, and derive the formula for the $2-$modified Fredholm determinant of $\mathcal{K}$ in terms of its kernel. We show that the eigenvalues of $\mathcal{L}$ are given by the zeros of the $2-$modified Fredholm determinant of $\mathcal{K}$.

In Section 4.6, we derive the conditions under which $\mathbf{K}$ is Lipschitz-continuous, and then finally in Section 4.7, we show that if these conditions hold, then $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R}, \mathbb{C}^4))$ is a trace class operator. Consequently, the regular Fredholm determinant of $\mathcal{K}$, $\det_1(\mathcal{I} + \mathcal{K}(\lambda))$, is defined, and in this situation, the eigenvalues of $\mathcal{L}$ are also given by the zeros of $\det_1(\mathcal{I} + \mathcal{K}(\lambda))$. In fact, using a result of [20], we see that $\det_1(\mathcal{I} + \mathcal{K}(\lambda))$ is equal to the Evans function. This allows us to locate the point spectrum of $\mathcal{L}$ using the zeros of the Fredholm determinant, rather than using the Evans function. The Evans function is defined in terms of the Jost solutions [20]. Although the Jost solutions have been shown to exist as solutions of a system of Volterra and Fredholm-type integral equations with exponential decay conditions [20], they are difficult to compute in practice. Numerically approximating the Fredholm determinant will prove much simpler. Additionally, we are able to quantify the error in the numerical approximation. In Section 4.8, we apply the error bounds we calculated in Sections 2.5 and 2.4 to the case of the CQ-CGLE.

In the next chapter, we will further specify these results on the CQ-CGLE to the case of the sech solution of the NLSE, so that we can test our theory numerically using this solution.

4.1 Linearization of the Complex Ginzburg-Landau Equation

We consider solutions of the cubic-quintic complex Ginzburg-Landau equation,

$$i\psi_t + \frac{D}{2}\psi_{xx} + \gamma|\psi|^2\psi + \nu|\psi|^4\psi = i\delta\psi + i\epsilon|\psi|^2\psi + i\beta\psi_{xx} + i\mu|\psi|^4\psi, \tag{4.3}$$

that are of the form

$$\psi(t,x) = \Psi(x)e^{-i\alpha t}, \tag{4.4}$$

for some phase change α. Then Ψ satisfies

$$i\Psi_t + \frac{D}{2}\Psi_{xx} + \gamma|\Psi|^2\Psi + \nu|\Psi|^4\Psi = (i\delta - \alpha)\Psi + i\epsilon|\Psi|^2\Psi + i\beta\Psi_{xx} + i\mu|\Psi|^4\Psi. \tag{4.5}$$

Assuming that at least one of $D, \beta \neq 0$, and letting $\mathbf{\Psi} = [\mathrm{Re}(\Psi)\ \ \mathrm{Im}(\Psi)]^T$, we can reformulate (4.5) as in [22] to obtain

$$\partial_t \mathbf{\Psi} = \left(\mathbf{B}\partial_x^2 + \mathbf{N}_0 + \mathbf{N}_1|\mathbf{\Psi}|^2 + \mathbf{N}_2|\mathbf{\Psi}|^4\right)\mathbf{\Psi}, \tag{4.6}$$

where

$$\mathbf{B} = \begin{bmatrix} \beta & -\frac{D}{2} \\ \frac{D}{2} & \beta \end{bmatrix}, \tag{4.7}$$

and

$$\mathbf{N}_0 = \begin{bmatrix} \delta & -\alpha \\ \alpha & \delta \end{bmatrix}, \quad \mathbf{N}_1 = \begin{bmatrix} \epsilon & -\gamma \\ \gamma & \epsilon \end{bmatrix}, \quad \mathbf{N}_2 = \begin{bmatrix} \mu & -\nu \\ \nu & \mu \end{bmatrix}. \tag{4.8}$$

Linearizing (4.6) about a stationary solution $\mathbf{\Psi}$, we obtain the equation

$$\partial_t \mathbf{p} = \mathcal{L}\mathbf{p}, \tag{4.9}$$

where

$$\mathcal{L} = \mathbf{B}\partial_x^2 + \widetilde{\mathbf{M}}, \tag{4.10}$$

with

$$\widetilde{\mathbf{M}}(x) = \mathbf{N}_0 + \mathbf{N}_1|\Psi|^2 + \mathbf{N}_2|\Psi|^4 + \left(2\mathbf{N}_1 + 4\mathbf{N}_2|\Psi|^2\right)\Psi\Psi^T. \tag{4.11}$$

Zweck et. al [22] show that if $\mathbf{\Psi}$ and its weak derivative $\mathbf{\Psi}_x$ are bounded on $\mathbb{R}$ and $\mathbf{\Psi}$ decays exponentially as $x \to \pm\infty$, then the linear operator

$$\mathcal{L} = \mathcal{L}(\mathbf{\Psi}(x)) : H^2(\mathbb{R}, \mathbb{C}^2) \subset L^2(\mathbb{R}, \mathbb{C}^2) \to L^2(\mathbb{R}, \mathbb{C}^2) \tag{4.12}$$

is closed, and therefore has a spectrum. The linear stability of the stationary pulse $\mathbf{\Psi}$ is determined by the spectrum of $\mathcal{L}$.

We recall [49], [50] that a linear operator, $\mathcal{L}$, on a Banach space, $\mathcal{X}$, is *Fredholm* if

1. $\mathrm{Ker}(\mathcal{L})$ is finite-dimensional, and

2. $R(\mathcal{L})$ is closed with finite co-dimension,

where $R(\mathcal{L})$ is the range of $\mathcal{L}$. The *Fredholm index* of such an operator is defined by

$$\mathrm{Ind}(\mathcal{L}) = \dim(\mathrm{Ker}(\mathcal{L})) - \mathrm{Codim}(R(\mathcal{L})). \tag{4.13}$$

The *resolvent set* of $\mathcal{L}$ is defined by

$$\rho(\mathcal{L}) := \{\lambda \in \mathbb{C} | (\mathcal{L} - \lambda\mathcal{I}) \text{ is invertible and } (\mathcal{L} - \lambda\mathcal{I})^{-1} \text{ is bounded}\}. \tag{4.14}$$

Then the *spectrum* of $\mathcal{L}$ is given by

$$\sigma(\mathcal{L}) := \mathbb{C} \setminus \rho(\mathcal{L}). \tag{4.15}$$

The *point spectrum* of $\mathcal{L}$ is defined by

$$\sigma_{\mathrm{pt}}(\mathcal{L}) := \{\lambda \in \mathbb{C} \,|\, \mathrm{Ker}(\mathcal{L} - \lambda\mathcal{I}) \neq \{0\}\}, \tag{4.16}$$

and the *Fredholm point spectrum* of $\mathcal{L}$ is the subset of $\sigma_{\mathrm{pt}}(\mathcal{L})$ such that

$$\sigma_{\mathrm{pt}}^{\mathcal{F}}(\mathcal{L}) := \{\lambda \in \mathbb{C} | (\mathcal{L} - \lambda\mathcal{I}) \text{ is Fredholm, } \mathrm{Ind}(\mathcal{L} - \lambda\mathcal{I}) = 0, \text{ and } \mathrm{Ker}(\mathcal{L} - \lambda\mathcal{I}) \neq 0\}. \tag{4.17}$$

Then the *essential spectrum* of $\mathcal{L}$ is defined by

$$\sigma_{\mathrm{ess}}(\mathcal{L}) := \sigma(\mathcal{L}) \setminus \sigma_{\mathrm{pt}}^{\mathcal{F}}(\mathcal{L}). \tag{4.18}$$

The spectrum of $\mathcal{L}$ is given by

$$\sigma(\mathcal{L}) = \sigma_{\mathrm{ess}}(\mathcal{L}) \cup \sigma_{\mathrm{pt}}(\mathcal{L}), \tag{4.19}$$

although this union may not be disjoint. Both the essential spectrum, σ_{ess}, and the point spectrum, σ_{pt}, of the operator $\mathcal{L}$ in (4.10) are computed with the aid of the asymptotic differential operator, $\mathcal{L}_\infty$. To define this operator, we assume that

$$\lim_{x\to\pm\infty} \|\Psi(x)\|_{\mathbb{C}^2} = 0, \tag{4.20}$$

so that

$$\mathbf{M}_\infty := \lim_{x\to\pm\infty} \widetilde{\mathbf{M}}(x) = \mathbf{N}_0. \tag{4.21}$$

As in Def. 3.1 in [22], the asymptotic differential operator $\mathcal{L}_\infty$ associated with $\mathcal{L}$ is defined by

$$\mathcal{L}_\infty = \mathbf{B}\partial_x^2 + \mathbf{M}_\infty = \mathbf{B}\partial_x^2 + \mathbf{N}_0. \tag{4.22}$$

To obtain the spectrum of the asymptotic operator $\mathcal{L}_\infty$, we convert the second-order differential equation $(\mathcal{L}_\infty - \lambda)\mathbf{p} = 0$ to the *unperturbed* first-order system

$$\partial_x \mathbf{Y} = \mathbf{A}_\infty(\lambda)\mathbf{Y}, \qquad \mathbf{Y} = [\mathbf{p} \;\; \mathbf{p}_x]^T, \tag{4.23}$$

where

$$\mathbf{A}_\infty(\lambda) = \begin{bmatrix} 0 & \mathbf{I} \\ \mathbf{B}^{-1}(\lambda - \mathbf{N}_0) & 0 \end{bmatrix}. \tag{4.24}$$

The operator $\mathcal{L}$ is a *relatively compact perturbation* of $\mathcal{L}_\infty$ [22], by which we mean that $\exists\lambda \in \rho(\mathcal{L}_\infty)$ such that $(\mathcal{L} - \mathcal{L}_\infty)(\mathcal{L}_\infty - \lambda\mathcal{I})^{-1} : \mathbb{R} \to \mathbb{R}$ is a compact operator. Then by Weyl's essential spectrum theorem [19], [22],

$$\sigma_{\text{ess}}(\mathcal{L}) = \sigma_{\text{ess}}(\mathcal{L}_\infty) = \sigma(\mathcal{L}_\infty) = \{\lambda \in \mathbb{C} \,|\, \exists\, \mu \in \mathbb{R} : \det[\mathbf{A}_\infty(\lambda) - i\mu] = 0\}. \tag{4.25}$$

In particular [22], we have that

$$\sigma_{\text{ess}}(\mathcal{L}_\infty) = \left\{ \lambda \in \mathbb{C} \,|\, \lambda = (\delta \pm i\alpha) - \mu^2 \left(\beta \pm i\frac{D}{2}\right) \text{ for some } \mu \in \mathbb{R} \right\}. \tag{4.26}$$

That is, $\lambda \in \sigma_{\text{ess}}(\mathcal{L}_\infty)$ if and only if the matrix $\mathbf{A}_\infty(\lambda)$ has a purely imaginary eigenvalue.

In Section 4.4, we will show that the point spectrum of $\mathcal{L}$ can be determined via an analysis of the related *perturbed* problem

$$\partial_x \mathbf{Y} = [\mathbf{A}_\infty(\lambda) + \mathbf{R}(x)]\mathbf{Y}, \tag{4.27}$$

where

$$\mathbf{R}(x) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ -\mathbf{B}^{-1}\mathbf{M}(x) & \mathbf{0} \end{bmatrix}, \tag{4.28}$$

with

$$\mathbf{M}(x) := \widetilde{\mathbf{M}}(x) - \mathbf{N}_0. \tag{4.29}$$

That is, $\lambda \in \sigma_{\mathrm{pt}}(\mathcal{L})$ if and only if (4.27) has a bounded solution. Knowledge of $\sigma(\mathbf{A}_\infty)$ will help determine these values of λ.

4.2 Diagonalization of the Unperturbed System

In this section, we calculate the spectrum of the matrix $\mathbf{A}_\infty(\lambda)$, defined in (4.24) where $\lambda \in \mathbb{C}$ is a given scalar.

We assume that at least one of β, D are nonzero, so that $\det(\mathbf{B}) \neq 0$. Then the matrix

$$\widehat{\mathbf{B}} = \begin{bmatrix} 0 & \mathbf{B} \\ \mathbf{B} & 0 \end{bmatrix} \tag{4.30}$$

is invertible. Premultiplying $\mathbf{A}_\infty - \sigma\mathbf{I}$ by $\widehat{\mathbf{B}}$ and applying the Schur determinant formula, we find that

$$\det\Big(\widehat{\mathbf{B}}(\mathbf{A}_\infty(\lambda) - \sigma\mathbf{I})\Big) = \det(\mathbf{B})\det\big(\lambda - \mathbf{N}_0 - \sigma^2\ \mathbf{B}\big). \tag{4.31}$$

Therefore, σ is an eigenvalue of $\mathbf{A}_\infty(\lambda)$ if and only if

$$\det\big(\lambda - \mathbf{N}_0 - \sigma^2\mathbf{B}\big) = 0, \tag{4.32}$$

since $\det(\mathbf{B}) \neq 0$. Since

$$\lambda - \mathbf{N}_0 - \sigma^2\mathbf{B} = \begin{bmatrix} \lambda - \delta - \sigma^2\beta & \alpha + \sigma^2\frac{D}{2} \\ -(\alpha + \sigma^2\frac{D}{2}) & \lambda - \delta - \sigma^2\beta \end{bmatrix}, \tag{4.33}$$

(4.32) holds if and only if

$$(\lambda - \delta - \sigma^2\beta)^2 = -\left(\alpha + \sigma^2\frac{D}{2}\right)^2, \tag{4.34}$$

which occurs when

$$\sigma^2 = \frac{\left[\beta(\lambda_R - \delta) - \frac{D}{2}(\alpha \pm \lambda_I)\right] + i\left[\beta(\lambda_I \pm \alpha) \pm \frac{D}{2}(\lambda_R - \delta)\right]}{\det(\mathbf{B})}, \tag{4.35}$$

where $\lambda = \lambda_R + i\lambda_I$.

Therefore, the eigenvalues of $\mathbf{A}_\infty(\lambda)$ are given by

$$\sigma_{1,\pm} = \pm\sqrt{R_1}e^{\frac{i\theta_1}{2}} \tag{4.36}$$

$$\sigma_{2,\pm} = \pm\sqrt{R_2}e^{\frac{i\theta_2}{2}}, \tag{4.37}$$

where

$$R_1 = \frac{\sqrt{\left[\beta(\lambda_R - \delta) - \frac{D}{2}(\alpha - \lambda_I)\right]^2 + \left[\beta(\lambda_I - \alpha) - \frac{D}{2}(\lambda_R - \delta)\right]^2}}{\det(\mathbf{B})}, \tag{4.38}$$

$$R_2 = \frac{\sqrt{\left[\beta(\lambda_R - \delta) - \frac{D}{2}(\alpha + \lambda_I)\right]^2 + \left[\beta(\lambda_I + \alpha) + \frac{D}{2}(\lambda_R - \delta)\right]^2}}{\det(\mathbf{B})}, \tag{4.39}$$

and

$$R_1\cos(\theta_1) = \frac{1}{\det(\mathbf{B})}\left[\beta(\lambda_R - \delta) - \frac{D}{2}(\alpha - \lambda_I)\right], \tag{4.40}$$

$$R_2\cos(\theta_2) = \frac{1}{\det(\mathbf{B})}\left[\beta(\lambda_R - \delta) - \frac{D}{2}(\alpha + \lambda_I)\right]. \tag{4.41}$$

Theorem 4.2.1. *Suppose that $(\beta, D) \neq (0,0)$ and $\lambda \notin \sigma_{ess}(\mathcal{L}_\infty)$. Then the matrix $\boldsymbol{A}_\infty(\lambda)$ has two eigenvalues with positive real part, and two eigenvalues with negative real part.*

Proof. Since σ_1, σ_2 are of the form (4.36), (4.37),

$$\sigma_{1,+} = -\sigma_{1,-} \tag{4.42}$$

$$\sigma_{2,+} = -\sigma_{2,-}, \tag{4.43}$$

and the matrix $\mathbf{A}_\infty$ will have the desired eigenvalue configuration unless the real part of at least one of $\sigma_{1,\pm}$ and $\sigma_{2,\pm}$ is zero. In this case, at least one of $\sigma_{1,\pm}$ and $\sigma_{2,\pm}$ is pure imaginary. Therefore, by (4.26), $\lambda \in \sigma_{\text{ess}}(\mathcal{L}_\infty)$, as $\lambda \in \sigma_{\text{ess}}(\mathcal{L}_\infty)$ if and only if $\mathbf{A}_\infty$ has a pure imaginary eigenvalue [22]. □

Next, we consider the conditions under which $\mathbf{A}_\infty(\lambda)$ has 4 distinct eigenvalues. Based on the results of the previous theorem, we make the following hypothesis.

Hypothesis 4.2.2. *The parameters in (4.3) and the scalar λ are assumed to satisfy the following conditions:*

1. $\beta \geq 0$,
2. $(\beta, D) \neq (0, 0)$,
3. $\lambda \notin \sigma_{ess}(\mathcal{L}_\infty)$.

Theorem 4.2.3. *Assume the conditions of Hypothesis 4.2.2. Then $\boldsymbol{A}_\infty(\lambda)$ has 4 distinct eigenvalues as given in (4.35), unless either*

1. $(D, \alpha) = (0, 0)$, *and if $\lambda \in \mathbb{R}, \lambda > \delta$, in which case, $\boldsymbol{A}_\infty(\lambda)$ has 2 repeated eigenvalues*

$$\sigma(\boldsymbol{A}_\infty) = \pm\sqrt{\frac{\lambda - \delta}{\beta}}, \tag{4.44}$$

or

2. $D \neq 0, \frac{\alpha}{D} < 0,$ *and* $\lambda = \frac{-2\alpha\beta}{D} + \delta,$ *in which case* $\boldsymbol{A}_\infty(\lambda)$ *has two repeated eigenvalues*

$$\sigma(\boldsymbol{A}_\infty) = \pm\sqrt{\frac{-2\alpha}{D}}. \tag{4.45}$$

Remark. *When* $\beta \neq 0$, *(4.45)is equivalent to (4.44).*

Proof. By Theorem 4.2.1, we know that $\mathbf{A}_\infty(\lambda)$ has two eigenvalues with positive real part and 2 with negative real part, so long as $(\beta, D) \neq (0,0)$ and $\lambda \notin \sigma_{\text{ess}}(\mathcal{L}_\infty)$. So these eigenvalues will be distinct unless

$$\sqrt{R_1}e^{i\frac{\theta_1}{2}} = \pm\sqrt{R_2}e^{i\frac{\theta_2}{2}}, \tag{4.46}$$

or equivalently, unless

$$R_1 e^{i\theta_1} = R_2 e^{i\theta_2}. \tag{4.47}$$

Equation (4.47) holds precisely when

$$R_1 \cos(\theta_1) = R_2 \cos(\theta_2), \tag{4.48}$$

$$R_1 \sin(\theta_1) = R_2 \sin(\theta_1). \tag{4.49}$$

By (4.40) and (4.41), we have that

$$R_1 \cos(\theta_1) = \frac{1}{\det(\mathbf{B})}(P + p), \tag{4.50}$$

$$R_2 \cos(\theta_2) = \frac{1}{\det(\mathbf{B})}(P - p), \tag{4.51}$$

where

$$P = \beta(\lambda_R - \delta) - \frac{D\alpha}{2}, \tag{4.52}$$

$$p = \frac{D}{2}\lambda_I. \tag{4.53}$$

Similarly,

$$R_1 \sin(\theta_1) = \frac{1}{\det(\mathbf{B})}(Q - q), \tag{4.54}$$

$$R_2 \sin(\theta_2) = \frac{1}{\det(\mathbf{B})}(Q + q), \tag{4.55}$$

where

$$Q = \beta\lambda_I, \tag{4.56}$$

$$q = \frac{D}{2}(\lambda_R - \delta) + \alpha\beta. \tag{4.57}$$

Therefore, (4.48) and (4.49) hold precisely when

$$P + p = P - p, \tag{4.58}$$

$$Q - q = Q + q, \tag{4.59}$$

which implies that $(p, q) = (0, 0)$. To examine the solutions of

$$\frac{D}{2}\lambda_I = 0, \tag{4.60}$$

$$\frac{D}{2}(\lambda_R - \delta) + \alpha\beta = 0, \tag{4.61}$$

we consider the two cases $D = 0$ and $D \neq 0$.

If $D = 0$, then $\beta \neq 0$ by assumption, so $\alpha = 0$ by (4.61). Therefore, by (4.35), we have that

$$\sigma^2 = \frac{\lambda - \delta}{\beta}. \tag{4.62}$$

If $\lambda \in \mathbb{R}$ and $\lambda \leq \delta$, then $\sigma^2 \leq 0$, so σ is pure imaginary and so $\lambda \in \sigma_{\text{ess}}(\mathcal{L}_\infty)$, contrary to our assumption. Therefore, if $\lambda \in \mathbb{R}$, then $\lambda > \delta$ must hold.

On the other hand, if $D \neq 0$, then $\lambda_I = 0$ by (4.60) and so, by (4.61), $\lambda - \delta = \frac{-2\alpha\beta}{D}$. Therefore, by (4.35), we find that

$$\begin{aligned} \sigma^2 &= \frac{\beta(\lambda - \delta) - \frac{\alpha D}{2} \pm i\left[\alpha\beta + \frac{D}{2}(\lambda - \delta)\right]}{\det \mathbf{B}} \\ &= \frac{\beta\left(\frac{-2\alpha\beta}{D}\right) - \frac{\alpha D}{2}}{\det \mathbf{B}}, \quad \text{by (4.61)} \\ &= \frac{\frac{-2\alpha}{D}\left[\beta^2 + \left(\frac{D}{2}\right)^2\right]}{\det \mathbf{B}} \\ &= \frac{-2\alpha}{D}. \end{aligned} \tag{4.63}$$

Since $D \neq 0$ by assumption, if $\frac{\alpha}{D} \geq 0$ we have

$$\sigma^2 = \frac{-2\alpha}{D} < 0, \tag{4.64}$$

so σ is pure imaginary and $\lambda \in \sigma_{\text{ess}}(\mathcal{L}_\infty)$, contrary to our hypothesis. Instead, we must assume that $\frac{\alpha}{D} < 0$ to get 2 repeated eigenvalues. □

By Theorem 4.2.3, when the eigenvalues of $\mathbf{A}_\infty$ are distinct, we can use the diagonalizability of the matrix to find the fundamental solutions of the differential equation (4.23). In the case where the eigenvalues are not distinct, we show that $\mathbf{A}_\infty$ is still diagonalizable.

Proposition 4.2.4. *Let* $a = \frac{\beta(\lambda-\delta)-\frac{D\alpha}{2}}{\det \boldsymbol{B}}$ *and* $b = -\frac{\frac{D}{2}(\lambda-\delta)-\beta\alpha}{\det \boldsymbol{B}}$. *If Hypothesis 4.2.2 holds, then* $\boldsymbol{A}_\infty(\lambda)$ *is diagonalizable, with*

$$\boldsymbol{A}_\infty(\lambda) = \begin{bmatrix} \boldsymbol{0}_{2\times 2} & \boldsymbol{I}_{2\times 2} \\ \boldsymbol{B}^{-1}(\lambda \boldsymbol{I} - \boldsymbol{N}_0) & \boldsymbol{0}_{2\times 2} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0}_{2\times 2} & \boldsymbol{I}_{2\times 2} \\ \begin{bmatrix} a & b \\ -b & a \end{bmatrix} & \boldsymbol{0}_{2\times 2} \end{bmatrix} = \boldsymbol{PDP}^{-1}, \tag{4.65}$$

and $a \pm bi \neq 0$, *since* $\lambda \notin \sigma_{ess}(\mathcal{L}_\infty)$ *by hypothesis. If* $\boldsymbol{A}_\infty$ *has distinct eigenvalues,*

$$\boldsymbol{P} = \begin{bmatrix} -i/\sqrt{a-bi} & i/\sqrt{a+bi} & -i/\sqrt{a+bi} & i/\sqrt{a-bi} \\ -1/\sqrt{a-bi} & -1/\sqrt{a+bi} & 1/\sqrt{a+bi} & 1/\sqrt{a-bi} \\ i & -i & -i & i \\ 1 & 1 & 1 & 1 \end{bmatrix}, \tag{4.66}$$

$$\boldsymbol{D} = \begin{bmatrix} -\sqrt{a-bi} & 0 & 0 & 0 \\ 0 & -\sqrt{a+bi} & 0 & 0 \\ 0 & 0 & \sqrt{a+bi} & 0 \\ 0 & 0 & 0 & \sqrt{a-bi} \end{bmatrix}, \tag{4.67}$$

and

$$\boldsymbol{P}^{-1} = \frac{1}{4}\begin{bmatrix} i\sqrt{a-bi} & -\sqrt{a-bi} & -i & 1 \\ -i\sqrt{a+bi} & -\sqrt{a+bi} & i & 1 \\ i\sqrt{a+bi} & \sqrt{a+bi} & i & 1 \\ -i\sqrt{a-bi} & \sqrt{a-bi} & -i & 1 \end{bmatrix}, \tag{4.68}$$

where $\sqrt{\cdot}$ *denotes the principal branch of the complex square root, and if, instead,* $\boldsymbol{A}_\infty$ *has 2 repeated eigenvalues,* σ_- *and* σ_+*, where* $\sigma_- = -\sigma_+$*, then*

$$\boldsymbol{P} = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & \sigma_- & 0 & \sigma_+ \\ \sigma_- & 0 & \sigma_+ & 0 \end{bmatrix}, \tag{4.69}$$

$$\boldsymbol{D} = \begin{bmatrix} \sigma_- & 0 & 0 & 0 \\ 0 & \sigma_- & 0 & 0 \\ 0 & 0 & \sigma_+ & 0 \\ 0 & 0 & 0 & \sigma_+ \end{bmatrix}, \tag{4.70}$$

and

$$\boldsymbol{P}^{-1} = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & 1/\sigma_- \\ 1 & 0 & 1/\sigma_- & 0 \\ 0 & 1 & 0 & 1/\sigma_+ \\ 1 & 0 & 1/\sigma_+ & 0 \end{bmatrix}. \tag{4.71}$$

Remark. *Note, additionally, that in both cases, the spectral projection* $\boldsymbol{Q}$ *onto the stable subspace of* $\boldsymbol{A}_\infty$ *is of the form* $\boldsymbol{Q} = \boldsymbol{P}\widehat{\boldsymbol{Q}}\boldsymbol{P}^{-1}$*, where*

$$\widehat{\boldsymbol{Q}} = \begin{bmatrix} \boldsymbol{I}_{2\times 2} & \boldsymbol{0}_{2\times 2} \\ \boldsymbol{0}_{2\times 2} & \boldsymbol{0}_{2\times 2}. \end{bmatrix} \tag{4.72}$$

Proof. Under the assumptions of the proposition, by (4.24), the spectrum of $\mathbf{A}_\infty$ is determined by its bottom-left block,

$$\mathbf{B}^{-1}(\lambda\mathbf{I}-\mathbf{N}_0)=\begin{bmatrix} a & b \\ -b & a\end{bmatrix}=\frac{1}{\det\mathbf{B}}\begin{bmatrix}\beta(\lambda-\delta)-\frac{\alpha D}{2} & \beta\alpha+\frac{D}{2}(\lambda-\delta) \\ -(\beta\alpha+\frac{D}{2}(\lambda-\delta)) & \beta(\lambda-\delta)-\frac{\alpha D}{2}\end{bmatrix}. \tag{4.73}$$

When $\mathbf{A}_\infty(\lambda)$ has 4 distinct eigenvalues, they are $\pm\sqrt{a\pm bi}$, and the diagonalization of $\mathbf{A}_\infty$ is given by (4.66)-(4.68). In the case where $\mathbf{A}_\infty$ has 2 repeated eigenvalues, $b=0$, and $\mathbf{A}_\infty$ takes the form

$$\mathbf{A}_\infty(\lambda)=\begin{bmatrix}\mathbf{0}_{2\times 2} & \mathbf{I}_{2\times 2} \\ \sigma^2\mathbf{I}_{2\times 2} & \mathbf{0}_{2\times 2}\end{bmatrix}, \tag{4.74}$$

where $\sigma^2=\frac{\lambda-\delta}{\beta}$, or $\sigma^2=\frac{-2\alpha}{D}$. The repeated eigenvalues are σ_-,σ_+, where $\mathrm{Re}\{\sigma_-\}<0<\mathrm{Re}\{\sigma_+\}$, and then the diagonalization of $\mathbf{A}_\infty$ is given by (4.69) - (4.71). □

Corollary 4.2.5. *In the case of the NLSE, where $\beta=\delta=\epsilon=\nu=\mu=0$, and $D=\gamma=1$,*

$$\boldsymbol{A}_\infty(\lambda)=\begin{bmatrix}0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -2\alpha & 2\lambda & 0 & 0 \\ -2\lambda & -2\alpha & 0 & 0\end{bmatrix}, \tag{4.75}$$

and by Theorem 4.2.3, under the assumptions of Hypothesis 4.2.2, $\boldsymbol{A}_\infty$ will have 4 distinct eigenvalues unless $\lambda=0$, and $\alpha<0$. When $\lambda=0,\alpha<0$, $\boldsymbol{A}_\infty(0)$ can be diagonalized as in

(4.69)-(4.71), with $\sigma_+ - \sqrt{-2\alpha}$. *In this case,*

$$\boldsymbol{P} = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & -\sqrt{-2\alpha} & 0 & \sqrt{-2\alpha} \\ -\sqrt{-2\alpha} & 0 & \sqrt{-2\alpha} & 0 \end{bmatrix}, \tag{4.76}$$

$$\boldsymbol{P}^{-1} = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & \frac{-1}{\sqrt{-2\alpha}} \\ 1 & 0 & \frac{-1}{\sqrt{-2\alpha}} & 0 \\ 0 & 1 & 0 & \frac{1}{\sqrt{-2\alpha}} \\ 1 & 0 & \frac{1}{\sqrt{-2\alpha}} & 0 \end{bmatrix}. \tag{4.77}$$

Alternatively, when $\lambda \neq 0$, $\boldsymbol{A}_\infty(\lambda)$ *is diagonalizable as in (4.66)-(4.68), with* $a = -2\alpha$ *and* $b = 2\lambda$, *where*

$$\boldsymbol{P} = \begin{bmatrix} \frac{-i}{\sqrt{2(-\alpha-i\lambda)}} & \frac{i}{\sqrt{2(-\alpha+i\lambda)}} & \frac{-i}{\sqrt{2(-\alpha+i\lambda)}} & \frac{i}{\sqrt{2(-\alpha-i\lambda)}} \\ \frac{-1}{\sqrt{2(-\alpha-i\lambda)}} & \frac{-1}{\sqrt{2(-\alpha+i\lambda)}} & \frac{1}{\sqrt{2(-\alpha+i\lambda)}} & \frac{1}{\sqrt{2(-\alpha-i\lambda)}} \\ i & -i & -i & i \\ 1 & 1 & 1 & 1 \end{bmatrix}, \tag{4.78}$$

$$\boldsymbol{P}^{-1} = \frac{1}{4}\begin{bmatrix} i\sqrt{2(-\alpha-i\lambda)} & -\sqrt{2(-\alpha-i\lambda)} & -i & 1 \\ -i\sqrt{2(-\alpha+i\lambda)} & -\sqrt{2(-\alpha+i\lambda)} & i & 1 \\ i\sqrt{2(-\alpha+i\lambda)} & \sqrt{2(-\alpha+i\lambda)} & i & 1 \\ -i\sqrt{2(-\alpha-i\lambda)} & \sqrt{2(-\alpha-i\lambda)} & -i & 1 \end{bmatrix}. \tag{4.79}$$

4.3 Bohl and Lyapunov Exponents for the Unperturbed Problem

In this section, we introduce the Bohl and Lyapunov exponents which quantify the exponential rates of decay of the stable and unstable solution spaces of the unperturbed problem (4.23). These exponents are used in the definitions and analysis of the Jost and Evans function.

The Bohl and Lyapunov exponents are defined for a general matrix $\mathbf{A}$ in [20]. Our purpose here is to calculate them for the matrix $\mathbf{A} = \mathbf{A}_\infty(\lambda)$ in Section 3.2. In particular, we exploit the fact that in this case, the ODE system (4.23) is autonomous and the matrix $\mathbf{A}$ is diagonalizable. We operate under the assumption that Hypothesis 4.2.2 is satisfied.

By Theorem 4.2.3 and Proposition 4.2.4, $\mathbf{A}$ can be diagonalized as

$$\mathbf{A} = \mathbf{A}_\infty(\lambda) = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}, \tag{4.80}$$

where $\mathbf{D}$ is the diagonal matrix containing the eigenvalues of $\mathbf{A}$, given by

$$\mathbf{D} = \begin{bmatrix} \sigma_{2,-} & 0 & 0 & 0 \\ 0 & \sigma_{1,-} & 0 & 0 \\ 0 & 0 & \sigma_{1,+} & 0 \\ 0 & 0 & 0 & \sigma_{2,+} \end{bmatrix}, \tag{4.81}$$

and $\mathbf{P}$ is given by (4.66) or (4.69).

Since $\mathbf{A}$ is x-independent, the fundamental matrix solution, $\mathbf{\Phi}$, of (4.23), is given by

$$\mathbf{\Phi}(x) = e^{\mathbf{A}x} = \mathbf{P}e^{\mathbf{D}x}\mathbf{P}^{-1}. \tag{4.82}$$

Consequently,

$$\mathbf{\Phi}^{-1}(x') = \mathbf{P}e^{-\mathbf{D}x'}\mathbf{P}^{-1}. \tag{4.83}$$

The Jost functions are defined in terms of the spectral projection, $\mathbf{Q}$, onto the stable subspace of $\mathbf{A}$, which is given by

$$\mathbf{Q} = \mathbf{P}\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\mathbf{P}^{-1}, \tag{4.84}$$

where $\mathbf{P}$ is a matrix of eigenvectors of $\mathbf{A}$. Because $\mathbf{Q}$ and $\mathbf{\Phi}$ are simultaneously diagonalizable, they commute. Therefore,

$$\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x') = \mathbf{\Phi}(x)\mathbf{Q}^2\mathbf{\Phi}^{-1}(x') = \mathbf{Q}e^{\mathbf{A}(x-x')}\mathbf{Q}, \tag{4.85}$$

and similarly,

$$\mathbf{\Phi}(x)(\mathbf{I}-\mathbf{Q})\mathbf{\Phi}^{-1}(x') = \mathbf{\Phi}(x)(\mathbf{I}-\mathbf{Q})^2\mathbf{\Phi}^{-1}(x') = (\mathbf{I}-\mathbf{Q})e^{\mathbf{A}(x-x')}(\mathbf{I}-\mathbf{Q}). \tag{4.86}$$

Following [20], we know that the propagator $\mathbf{\Phi}(x)\mathbf{\Phi}^{-1}(x')$ is *exponentially bounded* on $\mathbb{R}$, since $\exists C \in [1,\infty)$ and $\alpha \in \mathbb{R}$ so that

$$\|\mathbf{\Phi}(x)\mathbf{\Phi}^{-1}(x')\| \leq Ce^{\alpha(x-x')}, \quad \forall x, x' \in \mathbb{R}, \tag{4.87}$$

where $\|\cdot\|$ is the matrix 2-norm. We say that a projection $\mathbf{Q} \in \mathbb{C}^{4\times 4}$ is *uniformly conjugated* by $\mathbf{\Phi}$ on $\mathbb{R}$, if

$$\sup_{x\in\mathbb{R}} \|\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x)\| < \infty. \tag{4.88}$$

We recall the definitions of the Bohl and Lyapunov exponents associated with such a projection $\mathbf{Q}$. The *upper Bohl exponent*, $\varkappa(\mathbf{Q})$, on $\mathbb{R}$ is the infimum of all $\varkappa \in \mathbb{R}$ for which there exists $C(\varkappa) \in [1,\infty)$ such that

$$\|\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')\| \leq C(\varkappa)e^{\varkappa(x-x')} \quad \forall x \geq x'. \tag{4.89}$$

Similarly, the *lower Bohl exponent* $\varkappa'(\mathbf{Q})$ is the supremum of all $\varkappa \in \mathbb{R}$ for which the same condition holds but for all $x \leq x'$. Similarly, we can define upper and lower Bohl exponents on $\mathbb{R}_+$ and $\mathbb{R}_-$, denoted by $\{\varkappa_+(\mathbf{Q}), \varkappa'_+(\mathbf{Q})\}$ and $\{\varkappa_-(\mathbf{Q}), \varkappa'_-(\mathbf{Q})\}$, respectively [20, (2.6),(2.7)]. These Bohl exponents indicate the exponential rate of decay of the propagator $\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')$ over the specified domain, the upper exponent being the greatest rate of exponential growth and the lower exponent the least rate.

Similarly, we can define Lyapunov exponents which measure the greatest and least exponential growth rate of the fundamental solution, $\mathbf{\Phi}$, relative to $\mathbf{Q}$. For instance, the *upper Lyapunov exponent* associated with $\mathbf{Q}$ on $\mathbb{R}_+$ is given by

$$\lambda_+(\mathbf{Q}) = \limsup_{x\to\infty} \frac{\log \|\mathbf{\Phi}(x)\mathbf{Q}\|}{x}, \tag{4.90}$$

and the corresponding *lower Lyapunov exponent* is given by

$$\lambda'_+(\mathbf{Q}) = -\limsup_{x\to\infty} \frac{\log \|\mathbf{Q}\mathbf{\Phi}^{-1}(x)\|}{x}. \tag{4.91}$$

Furthermore, the projection $\mathbf{Q}$ is said to be an *exponential dichotomy* of (4.23) on $\mathbb{R}$ if for all $x, x' \in \mathbb{R}$, there exist positive constants $\varkappa, \varkappa', C(\varkappa), C(\varkappa')$ such that

$$\|\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')\| \leq C(\varkappa)e^{-\varkappa(x-x')},\ \forall x \geq x' \tag{4.92}$$

$$\|\mathbf{\Phi}(x)(\mathbf{I}-\mathbf{Q})\mathbf{\Phi}^{-1}(x')\| \leq C(\varkappa')e^{\varkappa'(x-x')},\ \forall x \leq x'. \tag{4.93}$$

Because it is autonomous, the system (4.23) has an exponential dichotomy, given by the spectral projection $\mathbf{Q}$ onto the stable space of $\mathbf{A}$ in (4.84).

We now compute the Bohl and Lyapunov exponents for the 4×4 matrix $\mathbf{A} = \mathbf{A}_\infty(\lambda)$ given by (4.24). We recall from (4.36), (4.37), and Theorem 4.2.3, that the eigenvalues of $\mathbf{A}$ are of the form

$$\sigma_{1,\pm} = \kappa_{1,\pm} + i\eta_{1,\pm} \tag{4.94}$$

$$\sigma_{2,\pm} = \kappa_{2,\pm} + i\eta_{2,\pm}, \tag{4.95}$$

where $\kappa_{j,-} = -\kappa_{j,+}$ and $\eta_{j,-} = -\eta_{j,+}$, for $j = 1, 2$. In addition,

$$\kappa_{2,-} \leq \kappa_{1,-} < 0 < \kappa_{1,+} \leq \kappa_{2,+}. \tag{4.96}$$

Theorem 4.3.1. *For a matrix, $\boldsymbol{A} = \boldsymbol{A}_\infty(\lambda)$, satisfying Hypothesis 4.2.2 which has eigenvalues with real parts satisfying (4.96), the upper Bohl and upper Lyapunov exponents associated with the projection $\boldsymbol{Q}$ given by (4.84) are*

$$\varkappa_\pm(\boldsymbol{Q}) = \lambda_\pm(\boldsymbol{Q}) = \kappa_{1,-}, \tag{4.97}$$

and the lower Bohl and lower Lyapunov exponents are

$$\varkappa'_\pm(\boldsymbol{Q}) = \lambda'_\pm(\boldsymbol{Q}) = \kappa_{2,-}. \tag{4.98}$$

The proof of this theorem depends on the following two lemmas.

Lemma 4.3.2. *For a matrix* $\boldsymbol{A}$ *satisfying Hypothesis 4.2.2, which has eigenvalues with real parts satisfying (4.96), we have that*

$$\varkappa_{\pm}(\boldsymbol{Q}) = \limsup_{(x-x')\to\infty} \frac{\ln \|\boldsymbol{\Phi}(x)\boldsymbol{Q}\boldsymbol{\Phi}^{-1}(x')\|}{x - x'} \geq \kappa_{1,-} \geq \kappa_{2,-}. \tag{4.99}$$

The proof of this Lemma can be found in Appendix 4.9.1.

Corollary 4.3.3. *Under the same conditions on* $\boldsymbol{A}$*,*

$$\lambda_{+}(\boldsymbol{Q}) = \limsup_{x\to\infty} \frac{\ln \|\boldsymbol{\Phi}(x)\boldsymbol{Q}\|}{x} \geq \kappa_{1,-} \geq \kappa_{2,-}, \tag{4.100}$$

and

$$\lambda_{-}(\boldsymbol{Q}) \leq \kappa_{1,-}. \tag{4.101}$$

Lemma 4.3.4. *For a matrix,* $\boldsymbol{A}$*, satisfying Hypothesis 4.2.2, which has eigenvalues with real parts satisfying (4.96), we have that*

$$\varkappa_{\pm}(\boldsymbol{Q}) \leq \kappa_{1,-}, \tag{4.102}$$

and that

$$\lambda_{\pm}(\boldsymbol{Q}) \leq \kappa_{1,-}. \tag{4.103}$$

The proof of this lemma can be found in Appendix 4.9.2.

Proof of Theorem 4.3.1. By Lemma 4.3.2, Corollary 4.3.3, and by Lemma 4.3.4, we have that

$$\varkappa_{\pm}(\mathbf{Q}) = \lambda_{\pm}(\mathbf{Q}) = \kappa_{1,-}. \tag{4.104}$$

To prove (4.98), we must show that each of $\varkappa'_{+}, \lambda'_{+} \geq \kappa_{2,-}$.

We have that

$$\begin{aligned}
\limsup_{(x-x')\to\infty} \frac{\ln\|\mathbf{\Phi}(x')\mathbf{Q}\mathbf{\Phi}^{-1}(x)\|}{x-x'} &= \limsup_{(x-x')\to\infty} \frac{\ln\|\mathbf{P}e^{-\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\mathbf{P}^{-1}\|}{x-x'} \\
&\leq \limsup_{(x-x')\to\infty} \frac{\ln\left[e^{\max\{-\kappa_{1,-}(x-x'),-\kappa_{2,-}(x-x')\}}\right]}{x-x'} \\
&= -\kappa_{2,-}, \qquad (4.105)
\end{aligned}$$

giving us that

$$\varkappa'_{+}(\mathbf{Q}) \geq \kappa_{2,-}, \qquad (4.106)$$

and thus that

$$\varkappa'_{+}(\mathbf{Q}) = \kappa_{2,-}. \qquad (4.107)$$

Similarly,

$$\begin{aligned}
\limsup_{x\to\infty} \frac{\ln\|\mathbf{Q}\mathbf{\Phi}^{-1}(x)\|}{x} &= \limsup_{x\to\infty} \frac{\ln\|\mathbf{P}e^{-\mathbf{D}x}\widehat{\mathbf{Q}}\mathbf{P}^{-1}\|}{x} \\
&\leq \limsup_{x\to\infty} \frac{\ln\left[e^{\max\{-\kappa_{1,-}x,-\kappa_{2,-}x\}}\right]}{x} \\
&= -\kappa_{2,-} \qquad (4.108)
\end{aligned}$$

giving us that

$$\lambda'_{\pm}(\mathbf{Q}) \geq \kappa_{2,-}, \qquad (4.109)$$

and thus that

$$\lambda'_{\pm}(\mathbf{Q}) = \kappa_{2,-}. \qquad (4.110)$$

This concludes the proof of the theorem. □

Corollary 4.3.5. *Suppose that Hypothesis 4.2.2 holds, and that the matrix, $\boldsymbol{A}$, has repeated eigenvalues with real parts $\kappa_- < 0 < \kappa_+$. Then the Bohl and Lyapunov exponents associated with the projection $\boldsymbol{Q}$ are all equal to κ_-.*

Proof. The proof for this case is identical to the case where $\kappa_{1,-} \geq \kappa_{2,-}$, (i.e. in Theorem 4.3.1), except that when eigenvalues are repeated, $\kappa_- := \kappa_{1,-} = \kappa_{2,-}$, all inequalities in the proof are given in terms of κ_-. That is,

$$\varkappa'_{\pm}(\mathbf{Q}) = \lambda'_{\pm}(\mathbf{Q}) = \kappa_- = \lambda_{\pm}(\mathbf{Q}) = \varkappa_{\pm}(\mathbf{Q}). \tag{4.111}$$

□

Next, we consider the exponential splitting of the projection $\mathbf{Q}$ in the case where the real parts of the eigenvalues are not equal [20]. When $\kappa_{1,-} \neq \kappa_{2,-}$, $\mathbf{A}$ has 4 distinct eigenvalues, and the exponential dichotomy projection, $\mathbf{Q}$, can be expressed as $\mathbf{Q} = \mathbf{Q}_{1,-} + \mathbf{Q}_{2,-}$, where $\mathbf{Q}_{1,-}$ and $\mathbf{Q}_{2,-}$ are spectral projections so that $\sigma(\mathbf{A}|_{\text{ran}(\mathbf{Q}_{j,-})}) = \sigma_{j,-}$ for $j = 1, 2$. Similarly, we have spectral projections $\mathbf{Q}_{1,+}$ and $\mathbf{Q}_{2,+}$ for which $\sigma(\mathbf{A}|_{\text{ran}(\mathbf{Q}_{j,+})}) = \sigma_{j,+}$ for $j = 1, 2$. We observe that

$$\mathbf{Q} = \mathbf{Q}_{1,-} + \mathbf{Q}_{2,-}, \tag{4.112}$$

and

$$\mathbf{I} - \ \mathbf{Q} = \mathbf{Q}_{1,+} + \mathbf{Q}_{2,+}. \tag{4.113}$$

Following [20], the system $\{\mathbf{Q}_{1,-}, \mathbf{Q}_{2,-}, \mathbf{Q}_{1,+}, \mathbf{Q}_{2,+}\}$ of such disjoint projections in $\mathbb{C}^4$ is an *exponential splitting* for (4.23) since the four Bohl segments $[\varkappa'(\mathbf{Q}_j), \varkappa(\mathbf{Q}_j)]$ are disjoint and $\mathbf{Q}_{1,-} + \mathbf{Q}_{2,-} + \mathbf{Q}_{1,+} + \mathbf{Q}_{2,+} = \mathbf{I}$.

Theorem 4.3.6. *Suppose that Hypothesis 4.2.2 holds and the matrix, $\boldsymbol{A}$, has distinct eigenvalues as described in (4.94), (4.95). Then, the Bohl and Lyapunov exponents for $\boldsymbol{Q}_j$ are all equal to $\kappa_{j,-}$, for $j = 1, 2$. That is,*

$$\varkappa_{\pm}(\boldsymbol{Q}_j) = \lambda_{\pm}(\boldsymbol{Q}_j) = \kappa_{j,-} = \varkappa'_{\pm}(\boldsymbol{Q}_j) = \lambda'_{\pm}(\boldsymbol{Q}_j). \tag{4.114}$$

Proof. Without loss of generality, consider the case where $j = 1$. Then

$$\mathbf{\Phi}(\boldsymbol{x})\mathbf{Q}_1\mathbf{\Phi}^{-1}(x') = \mathbf{P}\begin{bmatrix} \mathbf{E}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\mathbf{P}^{-1}, \tag{4.115}$$

where

$$\mathbf{E}_1 = \begin{bmatrix} e^{\kappa_{1,-}(x-x')} & 0 \\ 0 & 0 \end{bmatrix}. \tag{4.116}$$

By the method used in Theorem 4.3.2, we have that

$$\limsup_{(x-x')\to\infty} \frac{\ln \|\mathbf{\Phi}(x)\mathbf{Q}_1\mathbf{\Phi}^{-1}(x')\|}{x-x'} \geq \kappa_{1,-}. \tag{4.117}$$

Additionally, using the proof of Theorem 4.3.1, we also have that

$$\begin{aligned} \limsup_{(x-x')\to\infty} \frac{\ln \|\mathbf{\Phi}(x)\mathbf{Q}_1\mathbf{\Phi}^{-1}(x')\|}{x-x'} &\leq \limsup_{(x-x')\to\infty} \frac{\ln \left[\max\{e^{\kappa_{1,-}(x-x')}, 0\}\right]}{x-x'} \\ &= \limsup_{(x-x')\to\infty} \frac{\kappa_{1,-}(x-x')}{x-x'} \\ &= \kappa_{1,-}. \end{aligned} \tag{4.118}$$

Thus, we have that $\varkappa_+(\mathbf{Q}_1) = \kappa_{1,-}$, and that $\varkappa'_+(\mathbf{Q}_1) = \kappa_{1,-}$ as well. A similar argument holds for $\varkappa_-(\mathbf{Q}_1)$ and $\varkappa'_-(\mathbf{Q}_1)$. As for the Lyapunov exponents, we have that

$$\begin{aligned} \limsup_{x\to\infty} \frac{\ln \|\mathbf{\Phi}(x)\mathbf{Q}_1\|}{x} &\leq \limsup_{x\to\infty} \frac{\ln [\max\{e^{\kappa_{1,-}x}, 0\}]}{x} \\ &= \limsup_{x\to\infty} \frac{\kappa_{1,-}x}{x} \\ &= \kappa_{1,-}, \end{aligned} \tag{4.119}$$

and conversely, by Corollary 4.3.3,

$$\limsup_{x\to\infty} \frac{\ln \|\mathbf{\Phi}(x)\mathbf{Q}_1\|}{x} \geq \kappa_{1,-}. \tag{4.120}$$

Thus we have that

$$\lambda_+(\mathbf{Q}_1) = \kappa_{1,-}. \tag{4.121}$$

The same result holds for $\lambda'_+(\mathbf{Q}_1)$. Similarly, one can use the same argument to show that

$$\lambda_-(\mathbf{Q}_1) = \lambda'_-(\mathbf{Q}_1) = \kappa_{1,-}. \tag{4.122}$$

The proof for the case when $j = 2$ is identical. Thus, when working specifically with $\mathbf{Q}_j$, we have that all Bohl and Lyapunov exponents will be equivalent to $\kappa_{j,-}$. □

4.4 The Birman-Schwinger Operator for the Perturbed Problem

Throughout this section, we assume that the matrix $\mathbf{A} := \mathbf{A}_\infty(\lambda)$ satisfies Hypothesis 4.2.2. In particular, $\lambda \notin \sigma_{\text{ess}}(\mathcal{L})$. We observe that Hypothesis 2.8 of [20] holds for our constant matrix $\mathbf{A}_\infty$, and we assume that

$$\|\mathbf{R}\|_{\mathbb{C}^{4\times 4}} \in L^1(\mathbb{R}). \tag{4.123}$$

To characterize the spectrum of $\mathcal{L}$, we first define a first-order operator, $\mathcal{L}_A$, constructed from the second-order operator $\mathcal{L}_\infty$ in (4.22) such that $\sigma_{\text{ess}}(\mathcal{L}_A) = \sigma_{\text{ess}}(\mathcal{L}_\infty)$. Similarly, we define a first order-operator, $\mathcal{L}_{A+R}$, constructed from $\mathcal{L}$ in (4.10) such that $\lambda \in \sigma_{\text{pt}}(\mathcal{L}) \iff \text{Ker}(\mathcal{L}_{A+R}) \neq 0$. To do so, we let $\mathcal{L}_A, \mathcal{L}_{A+R} : H^1(\mathbb{R}, \mathbb{C}^4) \to L^2(\mathbb{R}.\mathbb{C}^4)$ be the operators associated with the unperturbed and perturbed systems (4.23) and (4.27), respectively; that is,

$$\begin{aligned} (\mathcal{L}_A \mathbf{u})(x) &:= -\mathbf{u}'(x) + \mathbf{A}\mathbf{u} &(4.124)\\ (\mathcal{L}_{A+R}\mathbf{u})(x) &:= (\mathcal{L}_A \mathbf{u})(x) + \mathbf{R}(x)\mathbf{u}. &(4.125)\end{aligned}$$

In particular, as is commonly assumed in the field, we expect that

$$\begin{aligned} \sigma_{\text{ess}}(\mathcal{L}_\infty) &= \sigma_{\text{ess}}(\mathcal{L}_A), &(4.126)\\ \sigma_{\text{pt}}(\mathcal{L}) &= \sigma_{\text{pt}}(\mathcal{L}_{A+R}), &(4.127)\end{aligned}$$

though this requires rigorous proof.

From the differential operator $\mathcal{L}_{A+R}$, we construct an integral operator, $\mathcal{K}(\lambda)$, which is a Green's function for (4.125). The operator $\mathcal{K}(\lambda)$ is defined using a construction originally due to Birman and Schwinger. We show that this operator is compact, and that $\lambda \in \sigma_{\text{pt}}(\mathcal{L})$ if and only if $\text{Ker}(\mathcal{I} + \mathcal{K}(\lambda)) \neq \{0\}$. In Section 4.5, we will show that the Birman-Schwinger operator $\mathcal{K}(\lambda)$ is Hilbert-Schmidt, and that under certain assumptions, is also trace class. We characterize the noninvertibility of $\mathcal{K}$ by showing that $\text{Ker}(\mathcal{L}_{A+R}) \neq 0$ when $\det_2(\mathcal{I}+\mathcal{K}(\lambda)) = 0$.

We begin by reviewing the derivation of the Green's operator, $\mathcal{G}_A$, for the unperturbed problem (4.124). Then we use $\mathcal{G}_A$ to obtain a solution operator for the perturbed problem (4.125). Finally, we use this solution operator to characterize the point spectrum of the operator $\mathcal{L}$ in (4.10).

First, we observe that $\mathbf{u} \in H^1(\mathbb{R}, \mathbb{C}^4)$ solves the unperturbed problem (4.124) on $\mathbb{R}$ if and only if $\mathbf{u} \in \text{Ker}(\mathcal{L}_A)$. By Hypothesis 4.2.2, none of the eigenvalues of $\mathbf{A}$ are pure imaginary. Consequently, nonzero solutions $\mathbf{u}(x) = e^{\mathbf{A}x}\mathbf{u}_0$ of (4.125) must grow as either $x \to \infty, x \to -\infty$, or both, and so cannot be in $L^2(\mathbb{R}, \mathbb{C}^4)$. Therefore, $\text{Ker}(\mathcal{L}_A) = \{0\}$.

Now, by the theory of exponential dichotomies [51], $\mathcal{L}_A$ is a Fredholm operator with Fredholm index 0. Therefore, since $\text{Ker}(\mathcal{L}_A) = \{0\}$, we also have that $\text{Coker}(\mathcal{L}_A) = \{0\}$. Hence, $\mathcal{L}_A$ is bijective and hence is invertible. In fact, we have an explicit formula for the Green's operator $\mathcal{G}_A = \mathcal{L}_A^{-1}$. Let

$$\mathbf{w} = \mathcal{L}_A\mathbf{u} = -\mathbf{u}' + \mathbf{A}\mathbf{u}, \quad \text{for } \mathbf{u} \in H^1. \tag{4.128}$$

Then

$$-e^{-\mathbf{A}x}\mathbf{w}(x) = e^{-\mathbf{A}x}\mathbf{u}'(x) - \mathbf{A}e^{-\mathbf{A}x}\mathbf{u}(x) = (e^{-\mathbf{A}x}\mathbf{u})'. \tag{4.129}$$

Now,

$$e^{-\mathbf{A}x}\mathbf{w}(x) = e^{-\mathbf{A}x}\mathbf{Q}\mathbf{w}(x) + e^{-\mathbf{A}x}(\mathbf{I} - \mathbf{Q})\mathbf{w}(x), \tag{4.130}$$

where $\mathbf{Q}$ is the projection operator onto the stable subspace of $\mathbf{A}$. Consequently,

$$\mathbf{u}(x)e^{-\mathbf{A}x} = \int_{-\infty}^{x} e^{-\mathbf{A}x'}\mathbf{Q}\mathbf{w}(x')dx' - \int_{x}^{\infty} e^{-\mathbf{A}x'}(\mathbf{I} - \mathbf{Q})\mathbf{w}(x')dx'. \tag{4.131}$$

Then

$$\mathbf{u}(x) = (\mathcal{G}_A\mathbf{w})(x) = \int_{\mathbb{R}} \mathbf{G}_A(x - x')\mathbf{w}(x')dx', \tag{4.132}$$

where

$$\mathbf{G}_A(x) = \begin{cases} -e^{\mathbf{A}x}\mathbf{Q}, & x \geq 0, \\ e^{\mathbf{A}x}(\mathbf{I}-\mathbf{Q}), & x \leq 0. \end{cases} \tag{4.133}$$

We note that $\mathbf{G}_A(x, x') := \mathbf{G}_A(x - x')$ belongs to $L^2(\mathbb{R} \times \mathbb{R}, \mathbb{C}^{4\times 4})$, since $\mathbf{G}_A(x) \to 0$ at an exponential rate as $x \to \pm\infty$. Therefore, $\mathcal{G}_A$ is a Hilbert Schmidt operator.

In the case that $\mathbf{A} = \mathbf{A}_\infty(\lambda)$ is given by (4.24), $\lambda \in \sigma_{\text{pt}}(\mathcal{L})$ if and only if $\text{Ker}(\mathcal{L}_{A+R}) \neq \{\mathbf{0}\}$. By the theory of exponential dichotomies [51], $\mathcal{L}_{A+R}$ is Fredholm of index 0, which implies that $\lambda \notin \sigma_{\text{pt}}(\mathcal{L})$ if and only if $\mathcal{L}_{A+R}$ is invertible. To find where $\mathcal{L}_{A+R}$ is invertible, we first consider the form of the perturbation operator, $\mathbf{R}$.

By (4.28), the perturbation operator, $\mathbf{R}(x)$, is given by

$$\mathbf{R}(x) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{T}(x) & \mathbf{0} \end{bmatrix}, \tag{4.134}$$

where $\mathbf{T}(x) = -\mathbf{B}^{-1}\mathbf{M}(x)$, with $\mathbf{M}(x)$ defined as in (4.11). We consider the polar decomposition of $\mathbf{R}(x)$, given by [35]

$$\mathbf{R}(x) = \mathbf{U}(x)|\mathbf{R}(x)|, \quad |\mathbf{R}(x)| = (\mathbf{R}(x)^*\mathbf{R}(x))^{1/2}, \quad x \in \mathbb{R}, \tag{4.135}$$

where $\mathbf{U}$ is unitary, and we define

$$\mathbf{R}_\ell(x) = \mathbf{U}(x)|\mathbf{R}(x)|^{1/2}, \quad \mathbf{R}_r(x) = |\mathbf{R}(x)|^{1/2}, \quad x \in \mathbb{R}, \tag{4.136}$$

and observe that

$$\mathbf{R}(x) = \mathbf{R}_\ell(x)\mathbf{R}_r(x). \tag{4.137}$$

Omitting the dependence on x for now, from (4.134), we have that

$$\mathbf{R}^* = \begin{bmatrix} \mathbf{0} & \mathbf{T}^* \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \tag{4.138}$$

and so

$$\mathbf{R}^*\mathbf{R} = \begin{bmatrix} \mathbf{S} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \tag{4.139}$$

where

$$\mathbf{S} = \mathbf{T}^*\mathbf{T} \tag{4.140}$$

is a normal, Hermitian matrix. Therefore, $\mathbf{S}$ is unitarily similar to the diagonal matrix containing its eigenvalues, i.e.

$$\mathbf{S} = \mathbf{W}\mathbf{D}_S\mathbf{W}^{-1}, \tag{4.141}$$

for some unitary matrix $\mathbf{W}$. Because $\mathbf{S}$ is Hermitian, its eigenvalues are real, and by (4.140), they are non-negative. Additionally, since $\mathbf{S} = \mathbf{T}^*\mathbf{T}$, we have that $\mathbf{S}^{1/2} = |\mathbf{T}|$. Therefore,

$$|\mathbf{R}| = (\mathbf{R}^*\mathbf{R})^{1/2} = \begin{bmatrix} |\mathbf{T}| & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}. \tag{4.142}$$

Now,

$$\begin{aligned} \mathbf{T}^*\mathbf{T} &= \mathbf{M}^T(\mathbf{B}^T)^{-1}\mathbf{B}^{-1}\mathbf{M} &(4.143)\\ &= \mathbf{M}^T(\mathbf{B}\mathbf{B}^T)^{-1}\mathbf{M} &(4.144)\\ &= (\det\mathbf{B})^{-1}\mathbf{M}^T\mathbf{M}, &(4.145) \end{aligned}$$

so

$$|\mathbf{T}| = (\det\mathbf{B})^{-1/2}|\mathbf{M}|, \tag{4.146}$$

and therefore,

$$|\mathbf{R}| = (\det\mathbf{B})^{-1/2}\begin{bmatrix} |\mathbf{M}| & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}. \tag{4.147}$$

Next, we claim that the unitary matrix, $\mathbf{U}$, in the polar decomposition of $\mathbf{R}$ in (4.135) is given by

$$\mathbf{U} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{T}|\mathbf{T}|^{-1} & \mathbf{0} \end{bmatrix}. \tag{4.148}$$

To see this, we observe that

$$\mathbf{U}|\mathbf{R}| = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{T}|\mathbf{T}|^{-1} & \mathbf{0} \end{bmatrix} \begin{bmatrix} |\mathbf{T}| & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{T} & \mathbf{0} \end{bmatrix} = \mathbf{R}. \tag{4.149}$$

Since $|\mathbf{T}|$ is Hermitian,

$$(\mathbf{T}|\mathbf{T}|^{-1})^*(\mathbf{T}|\mathbf{T}|^{-1}) = (|\mathbf{T}|^{-1})^*\mathbf{T}^*\mathbf{T}|\mathbf{T}|^{-1} = |\mathbf{T}|^{-1}\mathbf{S}|\mathbf{T}|^{-1} = \mathbf{I}. \tag{4.150}$$

Therefore, $\mathbf{U}$ is unitary, since

$$\mathbf{U}^*\mathbf{U} = \begin{bmatrix} \mathbf{0} & (\mathbf{T}|\mathbf{T}|^{-1})^* \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{T}|\mathbf{T}|^{-1} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} (\mathbf{T}|\mathbf{T}|^{-1})^*(\mathbf{T}|\mathbf{T}|^{-1}) & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} = \mathbf{I}. \tag{4.151}$$

Additionally,

$$\mathbf{U} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -(\det \mathbf{B})^{1/2}\mathbf{B}^{-1}\mathbf{V} & \mathbf{0} \end{bmatrix}, \tag{4.152}$$

where

$$\mathbf{V} = \mathbf{M}|\mathbf{M}|^{-1}. \tag{4.153}$$

So, we can write

$$\mathbf{R}_r = |\mathbf{R}|^{1/2} = (\det \mathbf{B})^{-1/4} \begin{bmatrix} |\mathbf{M}|^{1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \tag{4.154}$$

and

$$\mathbf{R}_\ell = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ -(\det \mathbf{B})^{1/4}\mathbf{B}^{-1}\mathbf{V}|\mathbf{M}|^{1/2} & \mathbf{0} \end{bmatrix}. \tag{4.155}$$

To simplify later calculations, we renormalize these matrices by redefining

$$\mathbf{R}_r := (\det \mathbf{B})^{1/4}|\mathbf{R}|^{1/2} = \begin{bmatrix} |\mathbf{M}|^{1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \tag{4.156}$$

and

$$\mathbf{R}_\ell := (\det \mathbf{B})^{-1/4}\mathbf{U}|\mathbf{R}|^{1/2} = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ -\mathbf{B}^{-1}\mathbf{M}|\mathbf{M}|^{-1/2} & \mathbf{0} \end{bmatrix}. \tag{4.157}$$

Applying the Birman-Schwinger principle [20], we observe that

$$\mathcal{L}_{A+R} = \mathcal{L}_A + \mathbf{R}, \tag{4.158}$$

$$= \mathcal{L}_A[\mathcal{I} + \mathcal{L}_A^{-1}\mathbf{R}] \tag{4.159}$$

$$= \mathcal{L}_A[\mathcal{I} + \mathcal{G}_A \mathbf{R}_\ell \mathbf{R}_r]. \tag{4.160}$$

From this, we obtain the following result.

Definition 4.4.1. *Let $\mathcal{L}$ be the differential operator associated with the perturbed problem (4.27). Let*

$$\mathcal{K}(\lambda) = \boldsymbol{R}_r \mathcal{G}_A(\lambda) \boldsymbol{R}_\ell, \tag{4.161}$$

$$\text{and } \widetilde{\mathcal{K}}(\lambda) = \mathcal{G}_A(\lambda) \boldsymbol{R}_\ell \boldsymbol{R}_r. \tag{4.162}$$

The unsymmetrized *and* symmetrized Birman-Schwinger operators *are defined to be the operators $\mathcal{I} + \widetilde{\mathcal{K}}(\lambda)$ and $\mathcal{I} + \mathcal{K}(\lambda)$.*

Theorem 4.4.2. *$\lambda \in \sigma_{pt}(\mathcal{L})$ if and only if the Birman-Schwinger operator $\mathcal{I} + \widetilde{\mathcal{K}}(\lambda)$ is not invertible.*

Proof. From (4.160), we see that $\mathcal{L}_{A+R}$ is invertible precisely when both $\mathcal{L}_A$ and $\mathcal{I} + \mathcal{G}_A \mathbf{R}_\ell \mathbf{R}_r$ are invertible. When $\lambda \notin \sigma_{\text{ess}}(\mathcal{L})$, $\mathcal{L}_A$ is always invertible. So $\mathcal{L}_{A+R}$ is not invertible if and only if $\mathcal{I} + \mathcal{G}_A \mathbf{R}_\ell \mathbf{R}_r$ is not invertible, and the result follows. □

4.5 Hilbert-Schmidt Kernel

In this section, we provide a condition on the perturbation, $\mathbf{R}$, which guarantees that the operators, $\mathcal{K}(\lambda)$ and $\widetilde{\mathcal{K}}(\lambda)$, are Hilbert-Schmidt operators. In the case of the operator $\mathcal{K}(\lambda)$, this result is as proved in [20]. Then, we state a theorem which characterizes λ, an eigenvalue of $\mathcal{L}$, as a zero of the 2−modified Fredholm determinant of $\mathcal{K}(\lambda)$. In particular, in contrast to the results in [22], we prove this result without any reference to the Evans function. In addition, we derive a bound on the Hilbert-Schmidt norm of $\mathcal{K}(\lambda)$ in terms of λ. As a corollary of this result, we also obtain a bound on the 2−modified Fredholm determinant of $\mathcal{K}(\lambda)$ in terms of λ.

Proposition 4.5.1. *Suppose that $\|\boldsymbol{R}\|_{\mathbb{C}^{4\times 4}} \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, where $\boldsymbol{R} = \boldsymbol{R}_\ell \boldsymbol{R}_r$ is decomposed as in (4.136). Define $\mathcal{K}$ and $\widetilde{\mathcal{K}}$ as in (4.161) and (4.162), respectively. Then both $\mathcal{K}$ and $\widetilde{\mathcal{K}}$ are in $\mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^4))$. Furthermore, the integral kernel of the operator $\mathcal{K}(\lambda)$ is given by*

$$\boldsymbol{K}(x, x'; \lambda) = \begin{cases} -\boldsymbol{R}_r(x)\,\boldsymbol{Q} e^{\boldsymbol{A}_\infty (x-x')}\,\boldsymbol{Q}\boldsymbol{R}_\ell(x'), & x \geq x', \\ \boldsymbol{R}_r(x)(\boldsymbol{I} - \boldsymbol{Q})e^{\boldsymbol{A}_\infty (x-x')}(\boldsymbol{I} - \boldsymbol{Q})\boldsymbol{R}_\ell(x'), & x < x', \end{cases} \tag{4.163}$$

where $\boldsymbol{A}_\infty$ and $\boldsymbol{Q}$ both depend on λ.

Proof. Since $\mathcal{K} = \mathbf{R}_r \mathcal{G}_A \mathbf{R}_\ell$, where $\mathcal{G}_A$ is defined in (4.132), the associated kernel $\mathbf{K}$ is given by

$$\mathbf{K}(x, x') = \begin{cases} -\mathbf{R}_r(x) e^{\mathbf{A}(x-x')}\mathbf{Q}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x) e^{\mathbf{A}(x-x')}(\mathbf{I} - \mathbf{Q})\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.164}$$

Expanding the fundamental solution as $e^{\mathbf{A}(x-x')} = \mathbf{\Phi}(x - x') = \mathbf{\Phi}(x)\mathbf{\Phi}^{-1}(x')$, we can write the kernel as

$$\mathbf{K}(x, x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{\Phi}(x)\mathbf{\Phi}^{-1}(x')\mathbf{Q}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)\mathbf{\Phi}(x)\mathbf{\Phi}^{-1}(x')(\mathbf{I} - \mathbf{Q})\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.165}$$

Furthermore, since the exponential dichotomy $\mathbf{Q}$ is a projection and since $\mathbf{Q}$ and $\mathbf{\Phi}$ are simultaneously diagonalizable and hence commute, we can rewrite the kernel as

$$\mathbf{K}(x, x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)\mathbf{\Phi}(x)(\mathbf{I} - \mathbf{Q})\mathbf{\Phi}^{-1}(x')\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.166}$$

Again using the commutativity of $\mathbf{\Phi}$ with projection $\mathbf{Q}$, we can finally write the kernel as

$$\mathbf{K}(x,x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(x-x')}\mathbf{Q}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(x-x')}(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.167}$$

By Lemma 2.9 in [20], since $\|\mathbf{R}\|_{\mathbb{C}^{4\times4}} \in L^1(\mathbb{R})$, $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R},\mathbb{C}^{4\times4}))$.

Similarly, the kernel $\widetilde{\mathbf{K}}$ for the operator $\widetilde{\mathcal{K}}$ is given by

$$\widetilde{\mathbf{K}}(x,x') = \begin{cases} -\mathbf{\Phi}(x)\mathbf{\Phi}^{-1}(x')\mathbf{Q}\mathbf{R}(x'),\ x \geq x', \\ \mathbf{\Phi}(x)\mathbf{\Phi}(x')(\mathbf{I}-\mathbf{Q})\mathbf{R}(x'),\ x < x'. \end{cases} \tag{4.168}$$

Now, since $\widetilde{\mathcal{K}} = \mathcal{G}_A\mathbf{R}$, the $\mathcal{J}_2-$norm of $\widetilde{\mathcal{K}}$ is given by

$$\|\widetilde{\mathcal{K}}\|_2^2 = \int_{\mathbb{R}} dx' \int_{x'}^{\infty} dx \|\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')\mathbf{R}(x')\|^2 \tag{4.169}$$

$$+ \int_{\mathbb{R}} dx' \int_{-\infty}^{x'} dx \|\mathbf{\Phi}(x)(\mathbf{I}-\mathbf{Q})\mathbf{\Phi}^{-1}(x')\mathbf{R}(x')\|^2. \tag{4.170}$$

Because $\mathbf{Q}$ is an exponential dichotomy, we know that

$$\|\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')\|^2 \leq Ce^{-\alpha(x-x')},\ \text{for } x \geq x', \tag{4.171}$$

$$\|\mathbf{\Phi}(x)(\mathbf{I}-\mathbf{Q})\mathbf{\Phi}^{-1}(x')\|^2 \leq De^{\beta(x-x')},\quad \text{for } x < x', \tag{4.172}$$

where $\alpha > 0$, $\beta > 0$, and $C, D \in [1,\infty)$. Therefore,

$$\begin{aligned} &\|\widetilde{\mathcal{K}}\|^2 \\ &\leq C\int_{\mathbb{R}} dx' \int_{x'}^{\infty} dx\ e^{-\alpha(x-x')}\|\mathbf{R}(x')\|^2 + D\int_{\mathbb{R}} dx' \int_{-\infty}^{x'} dx\ e^{\beta(x-x')}\|\mathbf{R}(x')\|^2 \\ &= C\int_{\mathbb{R}} dx' \left(e^{\alpha x'}\|\mathbf{R}(x')\|^2\right)\left[\frac{-1}{\alpha}\left(\lim_{t\to\infty} e^{-\alpha t} - e^{-\alpha x'}\right)\right] \\ &\quad +D\int_{\mathbb{R}} dx' \left(e^{-\beta x'}\|\mathbf{R}(x')\|^2\right)\left[\frac{1}{\beta}\left(\lim_{t\to-\infty} e^{\beta x'} - e^{\beta t}\right)\right] \\ &= \frac{-C}{\alpha}\int_{\mathbb{R}} dx'\|\mathbf{R}(x')\|^2 + \frac{D}{\beta}\int_{\mathbb{R}} dx'\|\mathbf{R}(x')\|^2 \\ &< \infty, \end{aligned} \tag{4.173}$$

since $\|\mathbf{R}\|_{\mathbb{C}^{4\times4}} \in L^2(\mathbb{R})$. Therefore, $\widetilde{\mathcal{K}} \in \mathcal{J}_2(L^2(\mathbb{R},\mathbb{C}^4))$. □

Hypothesis 4.5.2. *Let $\Psi = \Psi(x)$ be a stationary solution of the CQ-CGLE. Assume that $\exists\ \widetilde{C}, \widetilde{a} > 0$ such that*

$$|\Psi(x)| \leq \widetilde{C}e^{-\widetilde{a}|x|},\ \forall x \in \mathbb{R}. \tag{4.174}$$

Remark. *This hypothesis implies that the entries K_{ij} of the matrix-valued kernel $\boldsymbol{K}(x,y)$ in (4.163) also decay exponentially. One could use the constants $\widetilde{C}, \widetilde{a}$ to determine the constants C, a such that*

$$|K_{ij}(x,y)| \leq Ce^{-a(|x|+|y|)},\ \forall x, y \in \mathbb{R}. \tag{4.175}$$

Proposition 4.5.3. *Assume that Hypothesis 4.5.2 holds. Then $\mathcal{K}$ and $\widetilde{\mathcal{K}}$ as defined in (4.161) and (4.162) are Hilbert-Schmidt operators.*

Proof. By hypothesis,

$$|\Psi(x)| \leq \widetilde{C}e^{-\widetilde{a}|x|}, \forall x \in \mathbb{R}. \tag{4.176}$$

We recall that

$$\mathbf{R}(x) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ -\mathbf{B}^{-1}\mathbf{M}(x) & \mathbf{0} \end{bmatrix}, \tag{4.177}$$

where $\mathbf{B}$ is constant and $\mathbf{M}(x)$ depends on $\Psi(x)$. Since

$$\mathbf{M}(x) = \mathbf{N}_1|\Psi(x)|^2 + \mathbf{N}_2|\Psi(x)|^4 + (2\mathbf{N}_1 + 4\mathbf{N}_2|\Psi(x)|^2)\Psi\Psi^T, \tag{4.178}$$

$\|\mathbf{M}(x)\|$ decays exponentially whenever $|\Psi|$ does. Furthermore, since

$$\|\mathbf{R}(x)\| = \| - \mathbf{B}^{-1}\mathbf{M}(x)\| \leq \|\mathbf{B}^{-1}\|\|\mathbf{M}(x)\|, \tag{4.179}$$

this means that $\|\mathbf{R}\|$ will decay exponentially when $|\Psi|$ does. Because $\|\mathbf{R}(x)\|$ decays exponentially, $\|\mathbf{R}(x)\| \in (L^2 \cap L^2)(\mathbb{R})$, and so by Proposition 4.5.1, the result holds. □

Using Proposition 4.5.1, along with Proposition 2.3.11, we obtain the following theorem.

Theorem 4.5.4. *Suppose that* $\|\boldsymbol{R}\|_{\mathbb{C}^{4\times 4}} \in (L^1 \cap L^2)(\mathbb{R})$, *with* $\boldsymbol{R}$ *decomposed as in (4.136). Then*

$$\lambda \in \sigma_{\rm pt}(\mathcal{L}) \iff \det{}_2(\mathcal{I} + \mathcal{K}(\lambda)) = 0. \tag{4.180}$$

Proof. By Theorem 4.4.2,

$$\lambda \in \sigma_{\rm pt}(\mathcal{L}) \iff \mathcal{I} + \widetilde{\mathcal{K}} \text{ is not invertible}, \tag{4.181}$$

By Proposition 4.5.1, $\mathcal{K}, \widetilde{\mathcal{K}} \in \mathcal{J}_2$, and so by Proposition 2.3.11, we find that

$$\begin{aligned} \det{}_2(\mathcal{I} + \widetilde{\mathcal{K}}) &= \det{}_2(\mathcal{I} + (\mathcal{G}_A \mathbf{R}_\ell)\mathbf{R}_r) & (4.182)\\ &= \det{}_2(\mathcal{I} + \mathbf{R}_r(\mathcal{G}_A \mathbf{R}_\ell)) & (4.183)\\ &= \det{}_2(\mathcal{I} + \mathcal{K}). & (4.184) \end{aligned}$$

Finally, by Theorem 2.3.10,

$$\mathcal{I} + \widetilde{\mathcal{K}} \text{ is not invertible} \iff \det{}_2(\mathcal{I} + \widetilde{\mathcal{K}}) = 0, \tag{4.185}$$

and the result holds. □

Remark. *By [20, Theorem 8.3], we know that*

$$\det{}_2(\mathcal{I} + \mathcal{K}(\lambda)) = e^{\Theta(\lambda)} E(\lambda). \tag{4.186}$$

Here,

$$\Theta = \int_0^\infty \mathrm{Tr}(\boldsymbol{Q}\boldsymbol{R}(x))dx - \int_{-\infty}^0 \mathrm{Tr}((\boldsymbol{I} - \boldsymbol{Q})\boldsymbol{R}(x))dx, \tag{4.187}$$

where $\boldsymbol{Q} = \boldsymbol{Q}(\lambda)$ *is the projection onto the stable subspace of* $\boldsymbol{A} = \boldsymbol{A}(\lambda)$, *and*

$$E(\lambda) = \det(Y_+(0;\lambda) + Y_-(0;\lambda)), \tag{4.188}$$

where $Y_\pm = Y_\pm(x;\lambda)$ *are the matrix-valued Jost solutions* $Y_\pm$ *on* $\mathbb{R}_\pm$ *given in Definition 8.2 of [20]. By [20, Theorem 9.4],* $E(\lambda)$ *is precisely the Evans function for the stationary pulse* Ψ.

Equation (4.186) shows that the point spectrum of the pulse Ψ can be computed either by finding the zeros of the Evans function $E(\lambda)$ or the zeros of the $2-$modified Fredholm determinant of the Birman-Schwinger operator $\mathcal{I} + \mathcal{K}(\lambda)$.

Computational methods have been developed to calculate the Evans function [52]. The Jost functions are defined via a series of Volterra-type integrals, with exponential growth conditions along the boundaries, which makes them difficult to compute numerically. The main aim of this thesis is to investigate whether it is easier to compute values of $\det_2(\mathcal{I} + \mathcal{K}(\lambda))$ *instead of attempting to compute the Jost solutions.*

Since $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^4))$,

$$\|\mathcal{K}(\lambda)\|_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^{4\times 4}))} < \infty. \tag{4.189}$$

If we assume that $\mathbf{R}(x)$ decays exponentially as $x \to \pm\infty$, then we can obtain an upper bound for $\|\mathcal{K}(\lambda)\|_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^4))}$ as a function of λ.

Theorem 4.5.5. *Let $\mathcal{K} = \boldsymbol{R}_r \mathcal{G}_A(\lambda) \boldsymbol{R}_\ell \in \mathcal{J}_2(L^2(\mathbb{R}^2, \mathbb{C}^4))$ be the integral operator from Proposition 4.5.1, with $\boldsymbol{A}$ satisfying the hypotheses of Theorem 4.3.1, where $\|\boldsymbol{R}\| \in L^2(\mathbb{R}, \mathbb{C}^{4\times 4})$. Additionally, assume that*

$$\|\boldsymbol{R}(x)\| \leq C_R e^{-a|x|}, \tag{4.190}$$

for some $a, C_R > 0$. Then

$$\|\mathcal{K}(\lambda)\|^2_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^4))} \leq \frac{2C^2(\lambda)}{a^2}, \tag{4.191}$$

where

$$C(\lambda) = 4C_R \mathrm{cond}(\boldsymbol{P}(\lambda)). \tag{4.192}$$

Here, $\mathrm{cond}(\boldsymbol{P}(\lambda))$ *denotes the condition number of a matrix, $\boldsymbol{P}$, such that*

$$cond(\boldsymbol{P}(\lambda)) = \|\boldsymbol{P}(\lambda)\| \|\boldsymbol{P}^{-1}(\lambda)\| \tag{4.193}$$

measures the sensitivity of $\boldsymbol{P}$ to small changes in the parameter λ.

Remark. *Consequently, since by Theorem 2.3.10,* $\exists \Gamma > 0$ *such that*

$$|\det_2(\mathcal{I} + \mathcal{K}(\lambda))| \leq \exp\Big(\Gamma \|\mathcal{K}\|^2_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^4))}\Big), \tag{4.194}$$

we know that

$$|\det_2(\mathcal{I} + \mathcal{K}(\lambda))| \leq \exp\left(2\Gamma \frac{C^2(\lambda)}{a^2}\right) \tag{4.195}$$

is bounded, but the bound is dependent upon λ*.*

The proof of Theorem 4.5.5 relies on the following proposition.

Proposition 4.5.6.

$$\|\boldsymbol{Q} e^{\boldsymbol{A}_\infty (x-x')} \boldsymbol{Q}\|_{\mathbb{C}^{4\times 4}} \leq \sqrt{2}\,\mathrm{cond}(\boldsymbol{P}(\lambda)) e^{\kappa_{1,-}(x-x')},\ x \geq x', \tag{4.196}$$

$$\|(\boldsymbol{I} - \boldsymbol{Q}) e^{\boldsymbol{A}_\infty (x-x')} (\boldsymbol{I} - \boldsymbol{Q})\|_{\mathbb{C}^{4\times 4}} \leq \sqrt{2}\,\mathrm{cond}(\boldsymbol{P}(\lambda)) e^{\kappa_{1,+}(x-x')},\ x < x' \tag{4.197}$$

Proof of Proposition 4.5.6. When $x \leq x'$,

$$\begin{aligned}
\|\mathbf{Q} e^{\mathbf{A}_\infty(\lambda)(x-x')} \mathbf{Q}\|_{\mathbb{C}^{4\times 4}} &= \|\mathbf{P} \widehat{\mathbf{Q}} e^{\mathbf{D}(x-x')} \widehat{\mathbf{Q}} \mathbf{P}^{-1}\|_{\mathbb{C}^{4\times 4}} \\
&\leq \|\mathbf{P}\| \|\widehat{\mathbf{Q}} e^{\mathbf{D}(x-y)} \widehat{\mathbf{Q}}\| \|\mathbf{P}^{-1}\| \\
&\leq (\|\mathbf{P}\| \|\mathbf{P}^{-1}\|)\ \|\widehat{\mathbf{Q}} e^{\mathbf{D}(x-y)} \widehat{\mathbf{Q}}\|_F \\
&= \mathrm{cond}(\mathbf{P}) \|\widehat{\mathbf{Q}} e^{\mathbf{D}(x-y)} \widehat{\mathbf{Q}}\|_F \\
&= \mathrm{cond}(\mathbf{P}) \left(|e^{\sigma_{1,-}(x-x')}|^2 + |e^{\sigma_{2,-}(x-x')}|^2 \right)^{1/2} \\
&= \mathrm{cond}(\mathbf{P}) \left(e^{2\kappa_{1,-}(x-x')} + e^{2\kappa_{2,-}(x-x')} \right)^{1/2} \\
&\leq \sqrt{2}\,\mathrm{cond}(\mathbf{P}) e^{\kappa_{1,-}(x-x')},
\end{aligned} \tag{4.198}$$

where $\kappa_{2,-} \leq \kappa_{1,-} < 0$ by (4.96), and $\mathrm{cond}(\mathbf{P}) = \|\mathbf{P}\|\|\mathbf{P}^{-1}\|$ is the condition number of $\mathbf{P}(\lambda)$. Similarly, when $x < x'$,

$$\begin{aligned}
\|(\mathbf{I} - \mathbf{Q}) e^{\mathbf{A}_\infty(x-x')} (\mathbf{I} - \mathbf{Q})\| &\leq \mathrm{cond}(\mathbf{P}) \|(\mathbf{I} - \widehat{\mathbf{Q}}) e^{\mathbf{D}(x-x')} (\mathbf{I} - \widehat{\mathbf{Q}})\|_F \\
&= \mathrm{cond}(\mathbf{P}) \left(e^{2\kappa_{1,+}(x-x')} + e^{2\kappa_{2,+}(x-x')} \right)^{1/2} \\
&\leq \sqrt{2}\,\mathrm{cond}(\mathbf{P}) e^{\kappa_{1,+}(x-x')},
\end{aligned} \tag{4.199}$$

where $0 < \kappa_{1,+} \leq \kappa_{2,+}$ by (4.96). □

Proof of Theorem 4.5.5 . Recall that

$$(\mathcal{K}\mathbf{u})(\mathbf{x}) = \int_{\mathbb{R}} \mathbf{K}(x,x')\mathbf{u}(x')dx', \tag{4.200}$$

where

$$\mathbf{K}(x,x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(x-x')}\mathbf{Q}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(x-x')}(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.201}$$

As in [20, p. 373],

$$\begin{aligned} \|\mathcal{K}\|_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^4))} &= \int_{\mathbb{R}}\int_{\mathbb{R}} \|\mathbf{K}(x,x')\|^2_{\mathbb{C}^{4\times 4}} dx dx' \\ &= \int_{\mathbb{R}}\int_{-\infty}^{x} \|\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(\lambda)(x-x')}\mathbf{Q}\mathbf{R}_\ell(x')\|^2_{\mathbb{C}^{4\times 4}} dx' dx \\ &\quad + \int_{\mathbb{R}}\int_{x}^{\infty} \|\mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(\lambda)(x-x')}(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(x')\|^2_{\mathbb{C}^{4\times 4}} dx' dx \\ &\leq \int_{\mathbb{R}}\int_{-\infty}^{x} \|\mathbf{R}_r(x)\|^2\|\mathbf{R}_\ell(x')\|^2\|\mathbf{Q}e^{\mathbf{A}_\infty(\lambda)(x-x')}\mathbf{Q}\|^2 dx' dx \qquad (4.202) \\ &\quad + \int_{\mathbb{R}}\int_{x}^{\infty} \|\mathbf{R}_r(x)\|^2\|\mathbf{R}_\ell(x')\|^2\|(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(\lambda)(x-x')}(\mathbf{I}-\mathbf{Q})\|^2 dx' dx, \end{aligned}$$

which, since

$$\|\mathbf{R}_r\|^2 \leq \|\mathbf{R}\|, \|\mathbf{R}_\ell\|^2 \leq \|\mathbf{R}\|, \tag{4.203}$$

as in [20, p. 373], gives

$$\begin{aligned} \|\mathcal{K}\|^2_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^{d\times d}))} &\leq \int_{\mathbb{R}}\int_{-\infty}^{x} \|\mathbf{R}(x)\|\|\mathbf{R}(x')\|\|\mathbf{Q}e^{\mathbf{A}_\infty(\lambda)(x-x')}\mathbf{Q}\|^2 dx' dx \qquad (4.204) \\ &\quad + \int_{\mathbb{R}}\int_{x}^{\infty} \|\mathbf{R}(x)\|\|\mathbf{R}(x')\|\|(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(\lambda)(x-x')}(\mathbf{I}-\mathbf{Q})\|^2 dx' dx. \end{aligned}$$

Then by Proposition 4.5.6,

$$\begin{aligned} \|\mathcal{K}\|^2_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^{d}))} &\leq 2C_R^2\mathrm{cond}^2(\mathbf{P}(\lambda))\int_{\mathbb{R}}\int_{-\infty}^{x} e^{-a(|x|+|x'|)}e^{2\kappa_{1,-}(x-x')}dx' dx \\ &\quad +2C_R^2\mathrm{cond}^2(\mathbf{P}(\lambda))\int_{\mathbb{R}}\int_{x}^{\infty} e^{-a(|x|+|x'|)}e^{2\kappa_{1,+}(x-x')}dx' dx \\ &\leq 2C_R^2\mathrm{cond}^2(\mathbf{P}(\lambda))\int_{\mathbb{R}} e^{-\frac{a}{2}|x|}\int_{-\infty}^{x} e^{-\frac{a}{2}(|x|+|x'|)+2\kappa_{1,-}(x-x')}dx' dx \\ &\quad +2C_R^2\mathrm{cond}^2(\mathbf{P}(\lambda))\int_{\mathbb{R}} e^{-\frac{a}{2}|x|}\int_{x}^{\infty} e^{-\frac{a}{2}(|x|+|x'|)+2\kappa_{1,+}(x-x')}dx' dx. \qquad (4.205) \end{aligned}$$

Now, for $x' \leq x$,

$$-\frac{a}{2}(|x| + |x'|) \leq -\frac{a}{2}|x - x'| = -\frac{a}{2}(x - x'), \tag{4.206}$$

and similarly, for $x' \geq x$,

$$-\frac{a}{2}(|x| + |x'|) \leq -\frac{a}{2}(x' - x) = \frac{a}{2}(x - x'). \tag{4.207}$$

Therefore,

$$\begin{aligned} \|\mathcal{K}\|^2_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^d))} \leq \; & 2C_R^2\text{cond}^2(\mathbf{P}(\lambda)) \int_{\mathbb{R}} e^{-\frac{a}{2}|x|} \int_{-\infty}^{x} e^{-\left(\frac{a}{2} \mp 2\kappa_{1,-}(\lambda)\right)(x-x')} dx' dx \\ & +2C_R^2\text{cond}^2(\mathbf{P}(\lambda)) \int_{\mathbb{R}} e^{-\frac{a}{2}|x|} \int_{x}^{\infty} e^{\left(\frac{a}{2} + 2\kappa_{1,+}(\lambda)\right)(x-x')} dx' dx \\ = \; & \left[\frac{2C_R^2\text{cond}^2(\mathbf{P}(\lambda))}{\frac{a}{2} - 2\kappa_{1,-}(\lambda)} + \frac{2C_R^2\text{cond}^2(\mathbf{P}(\lambda))}{\frac{a}{2} + 2\kappa_{1,+}(\lambda)} \right] \int_{\mathbb{R}} e^{-\frac{a}{2}|x|} dx \\ = \; & \frac{4}{a} \left[\frac{2C_R^2\text{cond}^2(\mathbf{P}(\lambda))}{\frac{a}{2} - 2\kappa_{1,-}(\lambda)} + \frac{2C_R^2\text{cond}^2(\mathbf{P}(\lambda))}{\frac{a}{2} + 2\kappa_{1,+}(\lambda)} \right], \end{aligned} \tag{4.208}$$

since for $B > 0$,

$$\int_{-\infty}^{x} e^{-B(x-x')} dx' = \int_{x}^{\infty} e^{B(x-x')} dx' = \int_{0}^{\infty} e^{-By} dy = \frac{1}{B}. \tag{4.209}$$

So, since $\kappa_{1,+} = -\kappa_{1,-}$, the operator $\mathcal{K}$ is norm-bounded such that

$$\begin{aligned} \|\mathcal{K}(\lambda)\|^2_{\mathcal{B}_2(L^2(\mathbb{R},\mathbb{C}^d))} & \leq \frac{16C_R^2\text{cond}^2(\mathbf{P}(\lambda))}{a\left(\frac{a}{2} + 2\kappa_{1,+}(\lambda)\right)} \\ & \leq \frac{2C^2(\lambda)}{a^2}, \end{aligned} \tag{4.210}$$

with $C(\lambda) = 4C_R\text{cond}(\mathbf{P}(\lambda))$. The last inequality holds since for $a, \kappa_{1,+}(\lambda) \geq 0$, where we note that $\kappa_{1,+}(\lambda) = 0 \iff \lambda \in \sigma_{\text{ess}}(\mathcal{L}_\infty)$, by Theorem 4.2.1. □

4.6 Lipschitz Continuity of the Kernel

In order to apply Theorem 3.1.1 to show that $\mathcal{K}$ is trace class and to apply Theorem 2.5.3 to determine the rate of convergence of the numerical approximation of the Fredholm determinant $\det_p(\mathcal{I} + \mathcal{K})$, we must show that the kernel $\mathbf{K}$ is Lipschitz continuous.

We show that under suitable hypotheses on the pulse, Ψ, the elements of the matrix kernel $\mathbf{K}(x,y)$ are C^1 functions away from the diagonal $x=y$ and are continuous across the diagonal. Consequently, we can show that $\mathbf{K}(x,y)$ is Lipschitz-continuous on $[-L,L]\times[-L,L]$ for any $L<\infty$. Throughout this section, we suppose that the stationary pulse, Ψ, is C^1.

Recall that by Proposition 4.5.1,

$$\mathbf{K}(x,x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(x-x')}\mathbf{Q}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(x-x')}(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.211}$$

The main technical result of this section is a theorem which gives conditions on the parameters in the CQ-CGLE and on the pulse, Ψ, which guarantee that the kernel $\mathbf{K}(x,x')$ in (4.211) is C^1 on the sets $x<x'$ and $x>x'$. Significantly, $\mathbf{K}$ is also continuous across the diagonal, since

$$\begin{aligned} \lim_{x-x'\to 0^+}\mathbf{K}(x,x') &= \lim_{x-x'\to 0^+} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(x-x')}\mathbf{Q}\mathbf{R}_\ell(x') \\ &= -\mathbf{R}_r(x)\mathbf{Q}\mathbf{R}_\ell(x), \end{aligned} \tag{4.212}$$

as $\mathbf{Q}^2=\mathbf{Q}$, and

$$\begin{aligned} \lim_{x-x'\to 0^-}\mathbf{K}(x,x') &= \lim_{x-x'\to 0^-} \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(x-x')}(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(x') \\ &= \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(x) \\ &= \mathbf{R}_r(x)\mathbf{R}_\ell(x) - \mathbf{R}_r(x)\mathbf{Q}\mathbf{R}_\ell(x) \\ &= -\mathbf{R}_r(x)\mathbf{Q}\mathbf{R}_\ell(x), \end{aligned} \tag{4.213}$$

since $(\mathbf{I}-\mathbf{Q})^2=(\mathbf{I}-\mathbf{Q})$ and, most importantly, by (4.156), (4.157),

$$\mathbf{R}_r(x)\mathbf{R}_\ell(x) = \begin{bmatrix} |\mathbf{M}|^{1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ -\mathbf{B}^{-1}\mathbf{M}|\mathbf{M}|^{-1/2} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}. \tag{4.214}$$

However, $\mathbf{K}$ is not differentiable at points (x, x') where $x = x'$. Nevertheless, we will show that under suitable hypotheses, the entries of the matrix $\mathbf{K}(x, y)$ are Lipschitz continuous in both x and y. That is, for each $L > 0$, $\mathbf{K}_{ij}(x, y) \in C^{0,1}([-L, L]^2, \mathbb{C})$, $\forall i, j \in \{1, \ldots, 4\}$.

Since the matrices $\mathbf{R}_\ell$ and $\mathbf{R}_r$ are given in terms of $|\mathbf{M}|^{\pm 1/2} = (\mathbf{M}^*\mathbf{M})^{\pm 1/4}$, to show that $\mathbf{K}$ is C^1 on both $x > x'$ and $x < x'$, we must consider under what conditions the eigenvalues of $\mathbf{M}^*\mathbf{M}$ are distinct and non-zero. For if they are, then $|\mathbf{M}(x)|^{\pm 1/2}$ is C^1 in x. We begin with a general result valid for any $\mathbf{M} \in \mathbb{R}^{2\times 2}$ and then consider the matrix $\mathbf{M}$ that arises in the linearization of the CQ-CGLE.

Theorem 4.6.1. *Let $\boldsymbol{M}$ be any real 2×2 matrix. Assume that $\det(\boldsymbol{M}) > 0$ and that*

$$\frac{\operatorname{Tr}(\boldsymbol{M}^*\boldsymbol{M})}{2} - \det(\boldsymbol{M}) \neq 0. \tag{4.215}$$

Then the eigenvalues of $\boldsymbol{M}^*\boldsymbol{M}$ are distinct and nonzero.

Proof. First, we observe that if

$$\mathbf{M}^*\mathbf{M}\mathbf{v} = \lambda\mathbf{v} \;\text{ for } \mathbf{v} \neq 0, \tag{4.216}$$

then

$$\lambda = \frac{\|\mathbf{M}\mathbf{v}\|^2}{\|\mathbf{v}\|^2} \geq 0. \tag{4.217}$$

Moreover, since $\mathbf{M} \in \mathbb{R}^{2\times 2}$,

$$\det(\mathbf{M}^*\mathbf{M}) = [\det \mathbf{M}]^2 > 0, \tag{4.218}$$

which implies that both eigenvalues of $\mathbf{M}^*\mathbf{M}$ are positive, and so $\operatorname{Tr}(\mathbf{M}^*\mathbf{M}) > 0$. Since the eigenvalues of $\mathbf{M}^*\mathbf{M}$ are given by

$$\lambda_\pm(\mathbf{M}^*\mathbf{M}) = \frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2} \pm \sqrt{\left(\frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2}\right)^2 - \det(\mathbf{M}^*\mathbf{M})}, \tag{4.219}$$

they will be distinct provided that the discriminant

$$\left(\frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2}\right)^2 - \det(\mathbf{M}^*\mathbf{M}) \neq 0. \tag{4.220}$$

Since

$$\left(\frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2}\right)^2 - \det(\mathbf{M}^*\mathbf{M}) = \left(\frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2} - \det\mathbf{M}\right)\left(\frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2} + \det\mathbf{M}\right), \quad (4.221)$$

(4.220) holds if and only if

$$\frac{\operatorname{Tr}(\mathbf{M}^*\mathbf{M})}{2} - \det\mathbf{M} \neq 0, \quad (4.222)$$

since $\det(\mathbf{M}) > 0$ and $\operatorname{Tr}(\mathbf{M}^*\mathbf{M}) > 0$, and so the second factor on the right hand side of (4.221) is positive. □

We now apply Theorem 4.6.1 by calculating (4.222) for the matrix $\mathbf{M}$ given by

$$\mathbf{M} = \mathbf{N}_1|\boldsymbol{\psi}|^2 + \mathbf{N}_2|\boldsymbol{\psi}|^4 + (2\mathbf{N}_1 + 4\mathbf{N}_2|\boldsymbol{\psi}|^2)\boldsymbol{\psi}\boldsymbol{\psi}^T, \quad (4.223)$$

where $|\boldsymbol{\Psi}| := \|\boldsymbol{\Psi}(x)\|_2$. We observe that

$$\mathbf{M} = \mathbf{G} + \mathbf{H}\boldsymbol{\psi}\boldsymbol{\psi}^T, \quad (4.224)$$

where

$$\mathbf{G} \quad = \mathbf{N}_1|\boldsymbol{\psi}|^2 + \mathbf{N}_2|\boldsymbol{\psi}|^4 \quad = |\boldsymbol{\psi}|^2 \begin{bmatrix} \epsilon + \mu|\boldsymbol{\psi}|^2 & -(\gamma + \nu|\boldsymbol{\psi}|^2), \\ \gamma + \nu|\boldsymbol{\psi}|^2 & \epsilon + \mu|\boldsymbol{\psi}|^2 \end{bmatrix} \quad (4.225)$$

$$\mathbf{H} \quad = 2\mathbf{N}_1 + 4\mathbf{N}_2|\boldsymbol{\psi}|^2 \quad = \begin{bmatrix} 2\epsilon + 4\mu|\boldsymbol{\psi}|^2 & -(2\gamma + 4\nu|\boldsymbol{\psi}|^2) \\ 2\gamma + 4\nu|\boldsymbol{\psi}|^2 & 2\epsilon + 4\mu|\boldsymbol{\psi}|^2 \end{bmatrix}. \quad (4.226)$$

Letting $\alpha = \epsilon + \mu|\boldsymbol{\psi}|^2$ and $\beta = \gamma + \nu|\boldsymbol{\psi}|^2$, we have that

$$\mathbf{G} = |\boldsymbol{\psi}|^2 \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix}, \quad (4.227)$$

and

$$\mathbf{H} = \begin{bmatrix} 4\alpha - 2\epsilon & -(4\beta - 2\gamma) \\ 4\beta - 2\gamma & 4\alpha - 2\epsilon \end{bmatrix}. \quad (4.228)$$

Moreover,

$$\mathbf{G}^{-1} = \frac{1}{|\boldsymbol{\psi}|^2(\alpha^2+\beta^2)} \begin{bmatrix} \alpha & \beta \\ -\beta & \alpha \end{bmatrix}. \tag{4.229}$$

We calculate that

$$\det \mathbf{G} = |\boldsymbol{\psi}|^4(\alpha^2+\beta^2) = |\boldsymbol{\psi}|^4|\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2, \tag{4.230}$$

where

$$\mathbf{a} = \begin{bmatrix} \epsilon \\ \gamma \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} \mu \\ \nu \end{bmatrix}. \tag{4.231}$$

Since $\mathbf{M}$ is a rank one update of $\mathbf{G}$, by the Sherman-Morrison formula [35], we have that

$$\det \mathbf{M} = \det \mathbf{G}[1+\boldsymbol{\psi}^T\mathbf{G}^{-1}\mathbf{H}\boldsymbol{\psi}]. \tag{4.232}$$

A calculation shows that

$$\begin{aligned} \frac{\alpha^2+\beta^2}{2}\boldsymbol{\psi}^T\mathbf{G}^{-1}\mathbf{H}\boldsymbol{\psi} &= \alpha^2+\beta^2+|\boldsymbol{\psi}|^2(\alpha\mu+\beta\nu) \\ &= |\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2+|\boldsymbol{\psi}|^2(\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot\mathbf{b} \\ &= (\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot(\mathbf{a}+2|\boldsymbol{\psi}|^2\mathbf{b}), \end{aligned} \tag{4.233}$$

so that

$$1+\boldsymbol{\psi}^T\mathbf{G}^{-1}\mathbf{H}\boldsymbol{\psi} = 1+\frac{2}{\alpha^2+\beta^2}\left((\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot(\mathbf{a}+2|\boldsymbol{\psi}|^2\mathbf{b})\right), \tag{4.234}$$

and thus,

$$\det \mathbf{M} = |\psi|^4\left[3|\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2+2(\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot|\psi|^2\mathbf{b}\right]. \tag{4.235}$$

We can use a similar method to calculate $\frac{\mathrm{Tr}(\mathbf{M}^*\mathbf{M})}{2}$. By (4.224), we have that

$$\begin{aligned} \mathbf{M}^T\mathbf{M} &= (\mathbf{G}+\mathbf{H}\boldsymbol{\psi}\boldsymbol{\psi}^T)^T(\mathbf{G}+\mathbf{H}\boldsymbol{\psi}\boldsymbol{\psi}^T) \\ &= (\mathbf{G}^T+\boldsymbol{\psi}\boldsymbol{\psi}^T\mathbf{H}^T)(\mathbf{G}+\mathbf{H}\boldsymbol{\psi}\boldsymbol{\psi}^T) \\ &= \mathbf{G}^T\mathbf{G}+\boldsymbol{\psi}\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{G}+\mathbf{G}^T\mathbf{H}\boldsymbol{\psi}\boldsymbol{\psi}^T+\boldsymbol{\psi}\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{H}\boldsymbol{\psi}\boldsymbol{\psi}^T, \end{aligned} \tag{4.236}$$

and so,

$$\mathrm{Tr}(\mathbf{M}^*\mathbf{M}) = \mathrm{Tr}\big(\mathbf{G}^T\mathbf{G}\big) + 2\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{G}\boldsymbol{\psi} + |\boldsymbol{\psi}|^2\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{H}\boldsymbol{\psi}. \tag{4.237}$$

Now, from (4.227),

$$\begin{aligned}\mathrm{Tr}\big(\mathbf{G}^T\mathbf{G}\big) &= 2|\boldsymbol{\psi}|^4(\alpha^2+\beta^2)\\ &= 2|\boldsymbol{\psi}|^4|\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2.\end{aligned} \tag{4.238}$$

Additionally, using (4.225) and (4.226), we see that

$$\begin{aligned}2\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{G}\boldsymbol{\psi} &= 2\boldsymbol{\psi}^T(2\mathbf{N}_1+4\mathbf{N}_2|\boldsymbol{\psi}|^2)^T(\mathbf{N}_1|\boldsymbol{\psi}|^2+\mathbf{N}_2|\boldsymbol{\psi}|^4)\boldsymbol{\psi}\\ &= 4|\boldsymbol{\psi}|^2\left\{\boldsymbol{\psi}^T\mathbf{N}_1^T\mathbf{N}_1\boldsymbol{\psi}+|\boldsymbol{\psi}|^2\boldsymbol{\psi}^T\mathbf{N}_1^T\mathbf{N}_2\boldsymbol{\psi}\right.\\ &\quad\left.+2|\boldsymbol{\psi}|^2\boldsymbol{\psi}^T\mathbf{N}_2^T\mathbf{N}_1\boldsymbol{\psi}+2|\boldsymbol{\psi}|^4\boldsymbol{\psi}^T\mathbf{N}_2^T\mathbf{N}_2\boldsymbol{\psi}\right\}.\end{aligned} \tag{4.239}$$

Now,

$$\boldsymbol{\psi}^T\mathbf{N}_1^T\mathbf{N}_1\boldsymbol{\psi} = [\boldsymbol{\psi}_R\ \boldsymbol{\psi}_I]\begin{bmatrix}\epsilon^2+\gamma^2 & 0\\ 0 & \epsilon^2+\gamma^2\end{bmatrix}\begin{bmatrix}\boldsymbol{\psi}_R\\ \boldsymbol{\psi}_I\end{bmatrix} = (\epsilon^2+\gamma^2)|\boldsymbol{\psi}|^2 = |\mathbf{a}|^2|\boldsymbol{\psi}|^2, \tag{4.240}$$

and similarly,

$$\boldsymbol{\psi}^T\mathbf{N}_2^T\mathbf{N}_2\boldsymbol{\psi} = (\mu^2+\nu^2)|\boldsymbol{\psi}|^2 = |\mathbf{b}|^2|\boldsymbol{\psi}|^2. \tag{4.241}$$

Also,

$$\boldsymbol{\psi}^T\mathbf{N}_1^T\mathbf{N}_2\boldsymbol{\psi} = [\boldsymbol{\psi}_R\ \boldsymbol{\psi}_I]\begin{bmatrix}\epsilon\mu+\gamma\nu & \gamma\mu-\epsilon\nu\\ -\gamma\mu+\epsilon\nu & \epsilon\mu+\gamma\nu\end{bmatrix}\begin{bmatrix}\boldsymbol{\psi}_R\\ \boldsymbol{\psi}_I\end{bmatrix} = |\boldsymbol{\psi}|^2(\epsilon\mu+\gamma\nu) = |\boldsymbol{\psi}|^2(\mathbf{a}\cdot\mathbf{b}), \tag{4.242}$$

and hence,

$$\boldsymbol{\psi}^T\mathbf{N}_2^T\mathbf{N}_1\boldsymbol{\psi} = (\boldsymbol{\psi}^T\mathbf{N}_1^T\mathbf{N}_2\boldsymbol{\psi})^T = |\boldsymbol{\psi}|^2(\mathbf{a}\cdot\mathbf{b}). \tag{4.243}$$

So we have that

$$\begin{aligned}
2\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{G}\boldsymbol{\psi} &= 8|\boldsymbol{\psi}|^6(\mathbf{a}\cdot\mathbf{b}) + 8|\boldsymbol{\psi}|^8|\mathbf{b}|^2 + 4|\boldsymbol{\psi}|^4|\mathbf{a}|^2 + 4|\boldsymbol{\psi}|^6(\mathbf{a}\cdot\mathbf{b}) \\
&= 4|\boldsymbol{\psi}|^4\left[3|\boldsymbol{\psi}|^2(\mathbf{a}\cdot\mathbf{b}) + |\mathbf{a}|^2 + 2|\boldsymbol{\psi}|^4|\mathbf{b}|^2\right] \\
&= 4|\boldsymbol{\psi}|^4\left[3|\boldsymbol{\psi}|^2(\epsilon\mu+\gamma\nu) + (\epsilon^2+\gamma^2) + 2|\boldsymbol{\psi}|^4(\mu^2+\nu^2)\right] \\
&= 4|\boldsymbol{\psi}|^4\left[(\epsilon+|\boldsymbol{\psi}|^2\mu)^2 + (\gamma+|\boldsymbol{\psi}|^2\nu)^2\right] \\
&\quad +4|\boldsymbol{\psi}|^6\left[(\epsilon+|\boldsymbol{\psi}|^2\mu)\mu + (\gamma+|\boldsymbol{\psi}|^2\nu)\nu\right] \\
&= 4|\boldsymbol{\psi}|^4|\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2 + 4|\boldsymbol{\psi}|^6(\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot\mathbf{b} \qquad (4.244)
\end{aligned}$$

If we let $\zeta = 4\alpha - 2\epsilon$, and $\eta = 4\beta - 2\gamma$, then by (4.226),

$$\mathbf{H} = \begin{bmatrix} \zeta & -\eta \\ \eta & \zeta \end{bmatrix}, \qquad (4.245)$$

and so

$$\begin{aligned}
|\boldsymbol{\psi}|^2\boldsymbol{\psi}^T\mathbf{H}^T\mathbf{H}\boldsymbol{\psi} &= |\boldsymbol{\psi}|^2[\boldsymbol{\psi}_R\ \boldsymbol{\psi}_I]\begin{bmatrix} \zeta^2+\eta^2 & 0 \\ 0 & \zeta^2+\eta^2 \end{bmatrix}\begin{bmatrix} \boldsymbol{\psi}_R \\ \boldsymbol{\psi}_I \end{bmatrix} \\
&= |\boldsymbol{\psi}|^4(\zeta^2+\eta^2) \\
&= 4|\boldsymbol{\psi}|^4|\mathbf{a}+2|\boldsymbol{\psi}|^2\mathbf{b}|^2. \qquad (4.246)
\end{aligned}$$

Thus, by (4.237), (4.238), (4.239), and (4.246), we have that

$$\frac{\mathrm{Tr}(\mathbf{M}^*\mathbf{M})}{2} = 3|\boldsymbol{\psi}|^4|\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2 + 2|\boldsymbol{\psi}|^6(\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot\mathbf{b} + 2|\boldsymbol{\psi}|^4|\mathbf{a}+2|\boldsymbol{\psi}|^2\mathbf{b}|^2, \quad (4.247)$$

and therefore, by (4.235),

$$\frac{\mathrm{Tr}(\mathbf{M}^*\mathbf{M})}{2} - \det\mathbf{M} = 2|\boldsymbol{\psi}|^4|\mathbf{a}+2|\boldsymbol{\psi}|^2\mathbf{b}|^2. \qquad (4.248)$$

Proposition 4.6.2. *Consider the matrix* $\boldsymbol{M}$*, as defined in (4.223). Assume that* $\det\boldsymbol{M} > 0$*, and that either*

$$\epsilon + 2|\boldsymbol{\psi}|^2\mu \neq 0, \ \ \text{or}\ \gamma + 2|\boldsymbol{\psi}|^2\nu \neq 0. \qquad (4.249)$$

Then the eigenvalues of $\boldsymbol{M}^*\boldsymbol{M}$ *are distinct and nonzero.*

Proof. By Proposition 4.6.1, the eigenvalues of $\mathbf{M}$ will be distinct and nonzero, provided that

$$\frac{\mathrm{Tr}(\mathbf{M}^*\mathbf{M})}{2} - \det(\mathbf{M}) \neq 0, \tag{4.250}$$

where by (4.6.2),

$$\begin{aligned}\frac{\mathrm{Tr}(\mathbf{M}^*\mathbf{M})}{2} - \det(\mathbf{M}) &= 2|\boldsymbol{\psi}|^4|\mathbf{a} + 2|\boldsymbol{\psi}|^2\mathbf{b}|^2 &(4.251)\\ &= 2|\boldsymbol{\psi}|^4((\epsilon + 2|\boldsymbol{\psi}|^2\mu)^2 + (\gamma + 2|\boldsymbol{\psi}|^2\nu)^2). &(4.252)\end{aligned}$$

Now, since $|\boldsymbol{\psi}|$ is a factor of $\det \mathbf{M}$, which is assumed to be positive, (4.250) holds provided that

$$(\epsilon + 2|\boldsymbol{\psi}|^2\mu)^2 + (\gamma + 2|\boldsymbol{\psi}|^2\nu)^2 \neq 0, \tag{4.253}$$

which implies (4.249). □

Next, we formulate two hypotheses which together ensure that the eigenvalues of $\mathbf{M}^*(x)\mathbf{M}(x)$ are distinct and non-zero for all $x \in \mathbb{R}$.

Hypothesis 4.6.3. *Suppose that* $|\boldsymbol{\psi}(x)| > 0$ *for all* $x \in \mathbb{R}$. *Let*

$$\boldsymbol{a} = [\epsilon \quad \gamma]^T, \text{ and } \boldsymbol{b} = [\mu \quad \nu]^T. \tag{4.254}$$

Suppose that $\boldsymbol{a}$ *and* $\boldsymbol{b}$ *are not both* $\boldsymbol{0}$, *and that* $\epsilon \geq 0$ *and* $\gamma \geq 0$. *Assume that either* $\boldsymbol{a}$ *and* $\boldsymbol{b}$ *are linearly independent, or that if* $\boldsymbol{a} = m\boldsymbol{b}$ *for some* $m < 0$, *then*

$$\max_{x\in\mathbb{R}} |\boldsymbol{\psi}(x)|^2 < \frac{|m|}{2}. \tag{4.255}$$

Remark. *In the case of the NLSE, where* $\boldsymbol{b} = [\mu, \nu]^T = \boldsymbol{0}$ *and* $\boldsymbol{a} = [0, \gamma]^T$ *with* $\gamma > 0$, *Hypothesis 4.6.3 holds.*

Proposition 4.6.4. *Under the assumptions of Hypothesis 4.6.3,* $\mathrm{Tr}(\boldsymbol{M}^*\boldsymbol{M})/2 - \det(\boldsymbol{M}) \neq 0$ *for all* $x \in \mathbb{R}$.

Proof. By (4.251), we can guarantee that $\frac{\mathrm{Tr}(\mathbf{M}^*\mathbf{M})}{2} - \det(\mathbf{M}) \neq 0$ provided that

$$\mathbf{a} + 2|\boldsymbol{\psi}|^2\mathbf{b} \neq 0. \tag{4.256}$$

If $\mathbf{a}$ and $\mathbf{b}$ are linearly independent, then (4.256) holds. If one of $\mathbf{a}$ and $\mathbf{b}$ is zero, then (4.256) holds, since they are not both zero and $|\boldsymbol{\Psi}| > 0$. Therefore, we may assume that neither $\mathbf{a}$ nor $\mathbf{b}$ are zero and that they are linearly dependent. That is, we may assume

$$\mathbf{a} = m\mathbf{b}, \text{ for some } m \neq 0. \tag{4.257}$$

Since $\mathbf{a} \neq 0$, by the hypothesis, at least one of ϵ and γ is positive. Therefore, if $m > 0$, then either $\epsilon + 2|\boldsymbol{\psi}|^2\mu > 0$ or $\gamma + 2|\boldsymbol{\psi}|^2\nu > 0$, which implies that (4.256) holds. On the other hand, if $m < 0$, then at least one of μ, ν are strictly negative. Suppose $\mu < 0$. Since $\epsilon = m\mu$, we conclude that

$$\epsilon + 2|\boldsymbol{\psi}|^2\mu = (m + 2|\boldsymbol{\psi}|^2)\mu > 0, \tag{4.258}$$

by (4.255). Similarly, if $\nu < 0$, then $\gamma + 2|\boldsymbol{\psi}|^2\nu > 0$. So by (4.251), (4.256) holds for all $x \in \mathbb{R}$. □

Hypothesis 4.6.5. *Suppose that $|\boldsymbol{\psi}(x)| > 0\ \forall x \in \mathbb{R}$. Suppose that $\boldsymbol{a} = [\epsilon\ \gamma]^T$ and $\boldsymbol{b} = [\mu\ \nu]^T$ are not both $\boldsymbol{0}$, and that either $\boldsymbol{b} = \boldsymbol{0}$, or if $\boldsymbol{b} \neq \boldsymbol{0}$, let*

$$r_- := \frac{-4(\epsilon\mu + \gamma\nu) - \sqrt{16(\epsilon\mu + \gamma\nu)^2 - 15(\epsilon^2 + \gamma^2)(\mu^2 + \nu^2)}}{5(\mu^2 + \nu^2)}. \tag{4.259}$$

If r_- is real and positive, assume that

$$\max_{x \in \mathbb{R}} |\boldsymbol{\psi}(x)|^2 < r_-. \tag{4.260}$$

Proposition 4.6.6. *Under the assumptions of Hypothesis 4.6.5, we have that*

$$\det(\boldsymbol{M}(x)) > 0 \quad \forall x. \tag{4.261}$$

Proof. By (4.235),

$$\det \mathbf{M} = |\boldsymbol{\psi}|^4 \left[3|\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b}|^2 + 2(\mathbf{a}+|\boldsymbol{\psi}|^2\mathbf{b})\cdot|\boldsymbol{\psi}|^2\mathbf{b}\right]$$
$$= |\boldsymbol{\psi}|^4 \left[3|\mathbf{a}|^2 + 8|\boldsymbol{\psi}|^2\mathbf{a}\cdot\mathbf{b} + 5|\boldsymbol{\psi}|^4|\mathbf{b}|^2\right]. \quad (4.262)$$

Let

$$Q(t) = 3|\mathbf{a}|^2 + 8\mathbf{a}\cdot\mathbf{b}t + 5|\mathbf{b}|^2t^2. \quad (4.263)$$

By (4.262), it suffices to show that $Q(t) > 0$ for all $t \in \text{Im}(|\psi(x)|) := \{|\boldsymbol{\psi}(x)|\,|\,x \in \mathbb{R}\} \subset (0,\infty)$. If $\mathbf{b} = \mathbf{0}$, then $\mathbf{a} \neq \mathbf{0}$, and $Q(t) = 3|\mathbf{a}|^2 > 0$ for all $t \in \text{Im}(|\psi(x)|)$. If $\mathbf{a} = \mathbf{0}$, then $\mathbf{b} \neq \mathbf{0}$, and so $Q(t) = 5|\mathbf{b}|^2t^2 > 0$ for all $t \in \text{Im}(|\psi|)$. On the other hand, if $\mathbf{a} \neq \mathbf{0}$, then since $Q(0) = 3|\mathbf{a}|^2 > 0$ and $Q(t) \to \infty$ as $t \to \infty$, Q either has no positive roots, in which case $Q(t) > 0$, $\forall\, t > 0$, or Q has two positive roots. If Q has two positive roots, the smaller of these, r_-, is given by (4.259). Since $Q(t) > 0$ for all $t \in (0, r_-)$, $Q(|\boldsymbol{\psi}(x)|) > 0$ for all $x \in \mathbb{R}$ by (4.260).

Note: In the case of the NLSE, $\mathbf{b} = [\mu\ \nu]^T = \mathbf{0}$, and so when $|\psi(x)| > 0\,\forall x \in \mathbb{R}, \det(\mathbf{M}(x)) > 0$ as well. □

Combining these results, we obtain the main theorem in this section, which is a corollary to Theorem 3.1.1.

Theorem 4.6.7. *Suppose that* $\boldsymbol{\Psi} \in C^1(\mathbb{R}, \mathbb{C}^2)$, *that the kernel* $\boldsymbol{K}$ *given in (4.211) has the property that* $\boldsymbol{K}$ *and its first partial derivatives decay exponentially, and that both Hypothesis 4.6.3 and Hypothesis 4.6.5 hold. Then the kernel* $\boldsymbol{K}$ *is Lipschitz-continuous on* $[-L, L]^2$.

Proof. By Proposition 4.6.4, Proposition 4.6.6, and Theorem 4.6.1, the eigenvalues of $\mathbf{M}^*\mathbf{M}$ are distinct and positive. Therefore, the eigenvalues of $\mathbf{M}^*\mathbf{M}$, $|\mathbf{M}|^{1/2}$, and $|\mathbf{M}|^{-1/2}$ exist as C^1 functions of x. Since these matrices are 2×2, it is easy to show that the eigenfunctions of these operators can also be chosen to be C^1 functions of x. Therefore, $\mathbf{R}_\ell(x)$ and $\mathbf{R}_r(x)$ are C^1, and in addition, the solution operator $\mathbf{\Phi}(x) = e^{\mathbf{A}_\infty x}$ is C^1. Therefore,

$$|\mathbf{K}(x_1, y_1) - \mathbf{K}(x_2, y_2)| \leq M\|(x_1, y_1) - (x_2, y_2)\| \tag{4.264}$$

for all pairs of points $P = (x_1, y_1)$ and $Q = (x_2, y_2)$ that lie on the same side of the diagonal $y = x$.

To show that $\mathbf{K}$ is Lipschitz-continuous on all of $[-L, L]^2$, we just need to show that 4.264) also holds when the points P, Q lie on opposite sides of the diagonal. Let C be the line segment connecting P and Q and let $R = (x, x)$ be the point of intersection of this line segment with the diagonal. Let

$$\mathbf{K}(x, y) = \begin{cases} \mathbf{K}_-(x, y), & y \leq x, \\ \mathbf{K}_+(x, y), & y > x, \end{cases} \tag{4.265}$$

where $\mathbf{K}_\pm$ are given in terms of $\mathbf{R}_r(x), \mathbf{R}_\ell(y)$, and $\mathbf{\Phi}(x-y)$ by (4.165). Let $K(x, y) = K_{ij}(x, y)$ denote an entry of the matrix-valued kernel $\mathbf{K}(x, y)$. Since K_+ is C^1 on the compact set $[-L, L]^2$, $\|\nabla K_+\|$ is bounded on $[-L, L]^2$ and hence on $y < x$. Similarly, $\|\nabla K_-\|$ is bounded on $y > x$. So $\exists M > 0$ so that

$$\|\nabla K(x, y)\| \leq M, \ \forall (x, y) \in [-L, L]^2, \ \text{with } y \neq x. \tag{4.266}$$

Then by the fundamental theorem of calculus for line integrals,

$$K(x_1, y_1) = K_-(x, x) + \int_R^P \nabla K \cdot d\mathbf{r}, \tag{4.267}$$

where $y_1 < x_1$ and $K_-(x, x)$ is the limit of $K(x, y)$ as $(x, y) \to (x, x)$ from the left. Similarly,

$$K(x_2, y_2) = K_+(x, x) + \int_R^Q \nabla K \cdot d\mathbf{r}, \tag{4.268}$$

where $y_2 > x_2$ and $K_+(x,x)$ is the limite of $K(x,y)$ as $(x,y) \to (x,x)$ from the right. Since $\mathbf{K}$ is continuous across the diagonal, $K_+(x,x) = K_-(x,x)$, and so

$$\begin{aligned}
|K(x_1,y_1) - K(x_2,y_2)| &= \left| \int_R^P \nabla K \cdot d\mathbf{r} - \int_R^Q \nabla K \cdot d\mathbf{r} \right| \\
&\leq \left| \int_R^P \nabla K \cdot d\mathbf{r} \right| + \left| \int_R^Q \nabla K \cdot d\mathbf{r} \right| \\
&\leq M[\|(x_1,y_1) - (x,x)\| + \|(x_2,y_2) - (x,x)\|] \\
&= M\|(x_1,y_1) - (x_2,y_2)\|,
\end{aligned} \tag{4.269}$$

since R is on the line segment from P to Q. □

4.7 Trace Class Kernel

In this section, we apply the results from Chapter 3 to the specific case of the CQ-CGLE to understand under what conditions the Birman-Schwinger operator $\mathcal{K}$ is trace class. When $\mathcal{K}$ is trace class, we can deduce certain relationships between the trace of the Fredholm determinant $\det(\mathcal{I} + \mathcal{K})$, the 2-modified determinant $\det_2(\mathcal{I} + \mathcal{K})$, and the Evans function.

Theorem 4.7.1. *Let $\Psi(x)$ satisfy Hypotheses 4.6.3 and 4.6.5. Assume that Ψ satisfies Hypothesis 4.5.2 and additionally that*

$$|\Psi_x(x)| \leq \widetilde{C} e^{-\widetilde{a}|x|} \, \forall x \in \mathbb{R}, \tag{4.270}$$

for $\widetilde{C}, \widetilde{a} > 0$. Then $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R}, \mathbb{C}^4))$.

Proof. Since we assume that Ψ satisfies Hypotheses 4.6.3 and 4.6.5, the kernel $\mathbf{K}$ is Lipschitz-continuous by Theorem 4.6.7. Under the assumption of Hypothesis 4.5.2, along with the additional assumptions on the exponential decay of Ψ_x, we have that $\|\mathbf{K}\|, \|\partial_x \mathbf{K}\|$, and $\|\partial_y \mathbf{K}\|$ also decay exponentially, thus by Theorem 3.1.2, $\mathcal{K}$ is trace class. □

We recall from (4.186) that when $\mathcal{K} \in \mathcal{J}_2$,

$$\det{}_2(\mathcal{I} + \mathcal{K}(\lambda)) = e^{\Theta} E(\lambda), \tag{4.271}$$

where Θ is defined by (4.187) and $E(\lambda)$ is given in (4.188). If, additionally, $\mathcal{K}(\lambda) \in \mathcal{J}_1$, then $\mathrm{Tr}(\mathcal{K}(\lambda))$ and $\det(\mathcal{I} + \mathcal{K}(\lambda))$ are defined, and by Theorem 2.3.10,

$$\det{}_2(\mathcal{I} + \mathcal{K}(\lambda)) = e^{-\mathrm{Tr}(\mathcal{K})} \det(\mathcal{I} + \mathcal{K}(\lambda)). \tag{4.272}$$

We deduce the relation between Θ and $\mathrm{Tr}(\mathcal{K})$.

Proposition 4.7.2. *Suppose that $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R}, \mathbb{C}^k))$ is the Birman-Schwinger operator associated with the first order system*

$$\partial_x \boldsymbol{Y} = (\boldsymbol{A}_\infty(\lambda) + \boldsymbol{R}(x))\, \boldsymbol{Y}, \tag{4.273}$$

where $\mathrm{Tr}(\boldsymbol{R}(x)) = 0$. If, in addition, $\mathcal{K}$ is trace class, then

$$\mathrm{Tr}(\mathcal{K}) = -\Theta, \tag{4.274}$$

and

$$\det(\mathcal{I} + \mathcal{K}(\lambda)) = E(\lambda). \tag{4.275}$$

Proof. Recall from Proposition 4.5.1 that

$$\mathcal{K}\boldsymbol{\Psi}(x) = \int \mathbf{K}(x, x')\boldsymbol{\Psi}(x')dx', \tag{4.276}$$

where by (4.163) the kernel $\mathbf{K}(x, x')$ is given by

$$\mathbf{K}(x, x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(x-x')}\mathbf{Q}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)(\mathbf{I} - \mathbf{Q})e^{\mathbf{A}_\infty(x-x')}(\mathbf{I} - \mathbf{Q})\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{4.277}$$

Now, since $\mathcal{K}$ is trace class, we recall from (2.108) that

$$\mathrm{Tr}(\mathcal{K}) = \int_{\mathbb{R}} \mathrm{Tr}(\mathbf{K}(x, x))dx, \tag{4.278}$$

where $\mathbf{K}(x,x)$ is given by

$$\mathbf{K}(x,x) = -\mathbf{R}_r(x)\mathbf{Q}\mathbf{I}\mathbf{Q}\mathbf{R}_\ell(x) = -\mathbf{R}_r(x)\mathbf{Q}\mathbf{R}_\ell(x)dx. \tag{4.279}$$

Then, since $\operatorname{Tr}(\mathbf{AB}) = \operatorname{Tr}(\mathbf{BA})$,

$$\operatorname{Tr}(\mathcal{K}) = \int_{\mathbb{R}} \operatorname{Tr}(-\mathbf{R}_r(x)\mathbf{Q}\mathbf{R}_\ell(x))dx = -\int_{\mathbb{R}} \operatorname{Tr}(\mathbf{Q}\mathbf{R}_\ell(x)\mathbf{R}_r(x))dx = -\int_{\mathbb{R}} \operatorname{Tr}(\mathbf{Q}\mathbf{R}(x))dx. \tag{4.280}$$

Since $\operatorname{Tr}(\mathbf{R}(x)) = 0$, by [20, 8.12],

$$\Theta = \int_0^\infty \operatorname{Tr}(\mathbf{Q}\mathbf{R}(x))dx - \int_{-\infty}^0 \operatorname{Tr}((\mathbf{I}-\mathbf{Q})\mathbf{R}(x))dx = \int_{-\infty}^\infty \operatorname{Tr}(\mathbf{Q}\mathbf{R}(x))dx, \tag{4.281}$$

and thus $\theta = -\operatorname{Tr}(\mathcal{K})$. (4.275) now follows from (4.271) and (4.272). □

4.8 Error Bounds

In this section, we draw together the results in Chapters 2, 3, and 4 to formulate and prove the main theorem in this thesis. First, we recall that if a stationary pulse solution $\Psi = \Psi(x)$ of the CQ-CGLE satisfies Hypothesis 4.5.2, then the Birman-Schwinger operator $\mathcal{K}$ defined by (4.161) is a Hilbert-Schmidt operator on $\mathbb{R}$. Furthermore, if Ψ also satisfies the hypotheses in Theorem 4.7.1, then $\mathcal{K}$ is also a trace class operator on $\mathbb{R}$. Consequently, the Fredholm determinants $\det_p(\mathcal{I}+\mathcal{K}(\lambda))$ for $p = 1, 2$, are defined and their zeros can be used to determine the spectral stability of the pulse Ψ. In addition, in Sections 2.4, 2.5, we defined a matrix determinant approximation $d_{p,Q}(\lambda)$ of $\det_p(\mathcal{I} + \mathcal{K}(\lambda))$. This approximation was obtained by first truncating the domain of $\mathcal{K}(\lambda)$ to a compact interval $[-L, L]$ and then defining a block matrix discretization of the truncated operator in terms of a grid spacing of size Δx on the interval $[-L, L]$. We used the composite Simpson's quadrature rule on $[-L, L]$ with grid spacing Δx to derive the matrix determinant approximation $d_{p,Q}(\lambda)$ of $\det_p(\mathcal{I}+\mathcal{K}(\lambda))$. Specifically, we define $d_{p,Q}(\lambda)$ for $p = 1$ and 2 to be given by the formulae for $d_{1,Q}(z)$ in (2.272) and $d_{2,Q}(z)$ in (2.271) evaluated at $z = 1$.

By the results in Chapter 2, because our kernel is Lipschitz, we have the following bounds on the error between the Fredholm determinant $\det_p(\mathcal{I}+\mathcal{K})$ and our numerical approximation, $d_{p,Q}(\lambda)$.

Theorem 4.8.1. *Suppose that $\Psi = \Psi(x)$ is a stationary pulse solution of the CQ-CGLE which satisfies Hypothesis 4.5.2, and let $\mathcal{K} \in \mathcal{J}_2(L^2(\mathbb{R},\mathbb{C}^4))$ be the associated Birman-Schwinger operator, with matrix-valued kernel $\boldsymbol{K} \in (C^0 \cap L^2)(\mathbb{R},\mathbb{C}^{4\times 4})$ for which*

$$|K_{ij}(x,y)| \leq Ce^{-a(|x|+|y|)}, i,j \in 1,\ldots,4,\ \forall x,y \in \mathbb{R}. \tag{4.282}$$

Suppose that Ψ satisfies Hypotheses 4.6.3, and 4.6.5. Then

$$|\det_2(\mathcal{I}+\mathcal{K}(\lambda)) - d_{2,Q}(\lambda)| \leq e^{-aL}\boldsymbol{\Phi}\left(\frac{8C}{a}\right) + \frac{\sqrt{2\pi}e}{8}\Delta x \boldsymbol{\Phi}(8L\|\boldsymbol{K}\|_{W^{1,\infty}}), \tag{4.283}$$

where

$$\|\boldsymbol{K}\|_{W^{1,\infty}} = \max\{\|\partial_x \boldsymbol{K}\|_{L^\infty([a,b]^2,\mathbb{C}^{k\times k})}, \|\partial_y \boldsymbol{K}\|_{L^\infty([a,b]^2,\mathbb{C}^{k\times k})}, \|\boldsymbol{K}\|_{L^\infty([a,b]^2,\mathbb{C}^{k\times k})}\}. \tag{4.284}$$

In particular, the error in (4.283) converges to zero as $L \to \infty$ and $\Delta x \to 0$. If, in addition, Ψ satisfies the hypotheses of Theorem 4.7.1, then $\mathcal{K} \in \mathcal{J}_1(L^2(\mathbb{R},\mathbb{C}^4))$, and

$$|\det_1(\mathcal{I}+\mathcal{K}(\lambda)) - d_{1,Q}(\lambda)| \leq e^{-aL}\boldsymbol{\Phi}\left(\frac{8C}{a}\right) + \frac{\sqrt{2\pi}e}{8}\Delta x \boldsymbol{\Phi}(8L\|\boldsymbol{K}\|_{W^{1,\infty}}). \tag{4.285}$$

Proof. By the triangle inequality,

$$\begin{aligned} |\det_p(\mathcal{I}+z\mathcal{K}) - d_{p,Q}(\lambda)| \quad &\leq \quad |\det_p(\mathcal{I}+z\mathcal{K}) - \det_p(\mathcal{I}+\mathcal{K}|_{[-L,L]})| \\ &\quad + |\det_p(\mathcal{I}+\mathcal{K}|_{[-L,L]}) - d_{p,Q}(\lambda)|. \end{aligned} \tag{4.286}$$

The result now follows from Theorems 2.4.3 and 2.5.3. □

Remark. *Bornemann [26] shows that*

$$\boldsymbol{\Phi}(z) \leq z\boldsymbol{\Psi}(z\sqrt{2}e), \tag{4.287}$$

where

$$\boldsymbol{\Psi}(z) = 1 + \frac{\sqrt{\pi}}{2} z e^{z^2/4} \left[1 + \operatorname{erf}\left(\frac{z}{2}\right)\right]. \tag{4.288}$$

Additionally, if $z < 1$, then $\boldsymbol{\Phi}(z) < Dz$, for some constant D. Therefore, each of $\boldsymbol{\Phi}(8L\|\boldsymbol{K}\|_{W^{1,\infty}})$ and $\boldsymbol{\Phi}(8C/a)$ is bounded above by a constant depending on the decay and smoothness of $\boldsymbol{K}$.

To guarantee convergence of the approximated determinant to the true determinant, let $\epsilon > 0$. Then we can choose L sufficiently large so that

$$e^{-aL}\boldsymbol{\Phi}(8C/a) < \epsilon/2. \tag{4.289}$$

Then for this fixed L, we can calculate an appropriately small step size Δx so that

$$\frac{\sqrt{2\pi}e}{8}\Delta x \boldsymbol{\Phi}(8L\|\boldsymbol{K}\|_{W^{1,\infty}}) < \epsilon/2, \tag{4.290}$$

Then

$$|\det_p(\mathcal{I} + \mathcal{K}(\lambda)) - d_{p,Q}(\lambda)| < \epsilon. \tag{4.291}$$

4.9 Chapter 4 Appendix

4.9.1 Bohl and Lyapunov Exponents

Here we provide proofs about the Bohl and Lyapunov exponents of $\mathbf{Q}$, the projection matrix associated with the stable subspace of operator $\mathbf{A}_\infty$.

Lemma 4.9.1. *(Lemma 4.3.2) For a matrix $\boldsymbol{A}$ satisfying Hypothesis 4.2.2, which has eigenvalues with real parts satisfying (4.96), we have that*

$$\varkappa_\pm(\boldsymbol{Q}) = \limsup_{(x-x')\to\infty} \frac{\ln\|\boldsymbol{\Phi}(x)\boldsymbol{Q}\boldsymbol{\Phi}^{-1}(x')\|}{x - x'} \geq \kappa_{1,-} \geq \kappa_{2,-}. \tag{4.292}$$

Proof. Assume Hypothesis 4.2.2, and assume that $\mathbf{A}$ is diagonalizable and has eigenvalues with real parts satisfying (4.96). Then

$$\boldsymbol{\Phi}(x)\mathbf{Q}\boldsymbol{\Phi}^{-1}(x') = \mathbf{P}e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\mathbf{P}^{-1} = \mathbf{P}\begin{bmatrix} \mathbf{E} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\mathbf{P}^{-1}, \tag{4.293}$$

where

$$\mathbf{E} = \begin{bmatrix} e^{\kappa_{2,-}(x-x')} & 0 \\ 0 & e^{\kappa_{1,-}(x-x')} \end{bmatrix}. \tag{4.294}$$

We note that

$$\|\mathbf{A}\| \leq c\|\mathbf{P}\mathbf{A}\mathbf{P}^{-1}\| \tag{4.295}$$

for some $c \in \mathbb{R}$, since $\|\mathbf{A}_1\mathbf{A}_2\| \leq \|\mathbf{A}_1\|\|\mathbf{A}_2\|$. Furthermore, if $\mathbf{A} \in \mathbb{C}^{4\times 4}$,

$$\|\mathbf{A}\| \leq 2\|\mathbf{A}\|_F, \tag{4.296}$$

where $\|\cdot\|_F$ is the Frobenius norm. Then by (4.295), we have that

$$\begin{aligned}
\varkappa_+(\mathbf{Q}) = \limsup_{(x-x')\to\infty} \frac{\ln\|\boldsymbol{\Phi}(x)\mathbf{Q}\boldsymbol{\Phi}^{-1}(x')\|}{x-x'} &= \limsup_{(x-x')\to\infty} \frac{\ln\|\mathbf{P}e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\mathbf{P}^{-1}\|}{x-x'} \\
&\geq \limsup_{(x-x')\to\infty} \frac{\ln\left[\frac{1}{c}\|e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\|\right]}{x-x'} \\
&\geq \limsup_{(x-x')\to\infty} \frac{\ln\left[\frac{1}{2c}\|e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\|_F\right]}{x-x'} \\
&= \limsup_{(x-x')\to\infty} \frac{\ln\left[\frac{1}{2c}\right]}{x-x'} + \frac{\ln\|e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\|_F}{x-x'} \\
&= \limsup_{(x-x')\to\infty} \frac{\ln\|e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\|_F}{x-x'} \\
&= \limsup_{(x-x')\to\infty} \frac{\frac{1}{2}\ln\left[e^{2\kappa_{2,-}(x-x')} + e^{2\kappa_{1,-}(x-x')}\right]}{x-x'} \\
&\geq \limsup_{(x-x')\to\infty} \frac{\frac{1}{2}\ln\left[e^{2\kappa_{1,-}(x-x')}\right]}{x-x'}, \\
&= \limsup_{(x-x')\to\infty} \frac{\kappa_{1,-}(x-x')}{x-x'} \\
&= \kappa_{1,-} \geq \kappa_{2,-}.
\end{aligned} \tag{4.297}$$

The proof for $\varkappa_{-}(\mathbf{Q})$ is similar. □

Lemma 4.9.2. *(Lemma 4.3.4) For a matrix, $\boldsymbol{A}$, satisfying Hypothesis 4.2.2, which has eigenvalues with real parts satisfying (4.96), we have that*

$$\varkappa_{\pm}(\boldsymbol{Q}) \leq \kappa_{1,-}, \tag{4.298}$$

$$\textit{and } \lambda_{\pm}(\boldsymbol{Q}) \leq \kappa_{1,-}. \tag{4.299}$$

Proof. For the upper Bohl exponent, $\varkappa_{+}(\mathbf{Q})$, since the matrix 2-norm satisfies $\|\mathbf{A}_1\mathbf{A}_2\| \leq \|\mathbf{A}_1\|\|\mathbf{A}_2\|$, we have that

$$\begin{aligned}
\varkappa_{+}(\mathbf{Q}) &= \limsup_{(x-x')\to\infty} \frac{\ln\|\mathbf{\Phi}(x)\mathbf{Q}\mathbf{\Phi}^{-1}(x')\|}{x-x'} \\
&= \limsup_{(x-x')\to\infty} \frac{\ln\|\mathbf{P}e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\mathbf{P}^{-1}\|}{x-x'} \\
&\leq \limsup_{(x-x')\to\infty} \frac{\ln\|\mathbf{P}\| + \ln\|\mathbf{P}^{-1}\|}{x-x'} + \frac{\ln\|e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\|}{x-x'} \\
&= \limsup_{(x-x')\to\infty} \frac{\ln\|e^{\mathbf{D}(x-x')}\widehat{\mathbf{Q}}\|}{x-x'} \\
&= \limsup_{(x-x')\to\infty} \frac{\ln\left[e^{\max\{\kappa_{1,-}(x-x'),\kappa_{2,-}(x-x')\}}\right]}{x-x'} \\
&= \limsup_{x-x'\to\infty} \frac{\kappa_{1,-}(x-x')}{x-x'} \\
&= \kappa_{1,-}.
\end{aligned} \tag{4.300}$$

Similarly, $\varkappa_-(\mathbf{Q}) \leq \kappa_{1,-}$. As for the upper Lyapunov exponent, $\lambda_+(\mathbf{Q})$, we have that

$$\begin{aligned}
\lambda_+(\mathbf{Q}) &= \limsup_{x\to\infty} \frac{\ln \|\mathbf{\Phi}(x)\mathbf{Q}\|}{x} \\
&= \limsup_{x\to\infty} \frac{\ln \|\mathbf{P}e^{\mathbf{D}x}\widehat{\mathbf{Q}}\mathbf{P}^{-1}\|}{x} \\
&\leq \limsup_{x\to\infty} \frac{\ln \|e^{\mathbf{D}x}\widehat{\mathbf{Q}}\|}{x} \\
&= \limsup_{x\to\infty} \frac{\ln \left[e^{\max\{\kappa_{1,-}x,\kappa_{2,-}x\}}\right]}{x} \\
&= \limsup_{x\to\infty} \frac{\kappa_{1,-}x}{x} \\
&= \kappa_{1,-}.
\end{aligned} \tag{4.301}$$

A similar calculation shows that $\lambda_-(\mathbf{Q}) \leq \kappa_{1,-}$. □

CHAPTER 5

NUMERICAL RESULTS FOR THE SECH SOLUTION OF THE NLSE

The sech pulse is a well-known soliton solution to the nonlinear Schrodinger equation (NLSE). In this section, we study the Hilbert-Schmidt operator $\mathcal{K}$ associated with this solution. In particular, we explicitly calculate the matrix-valued kernel $\mathbf{K}(x, y)$ in this case, and we apply the results from Chapters 2, 3 and 4 to this kernel. We show that the hypotheses used in the theory apply to the sech solution of the NLSE and that $\mathcal{K}$ is, in fact, trace class, and we explicitly calculate bounds on the error between the regular Fredholm determinant of $\mathcal{K}$ and our numerical approximation. Finally, we present numerical results that validate the theory developed in the Chapters 2, 3, and 4.

5.1 Kernel of the NLSE

Recall that the NLSE is the special case of the CGLE for which the parameters are given by

$$\beta = \delta = \epsilon = \mu = \nu = 0, \text{ and } \gamma > 0. \tag{5.1}$$

To obtain a sech solution of the NLSE, we need $D > 0$. To simplify the discussion, and without any further loss of generality, we set $\gamma = D = 1$. Therefore,

$$\mathbf{B} = \begin{bmatrix} 0 & -\frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix}, \tag{5.2}$$

and

$$\mathbf{N}_0 = \begin{bmatrix} 0 & \frac{1}{2} \\ -\frac{1}{2} & 0 \end{bmatrix}, \quad \mathbf{N}_1 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{N}_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}. \tag{5.3}$$

Then

$$\psi(t, x) = \operatorname{sech}(x) e^{it/2} \tag{5.4}$$

solve the NLSE, and so we set

$$\Psi(x) = \operatorname{sech}(x), \tag{5.5}$$

and $\alpha = -1/2$ in the CQ-CGLE in (4.3). Then

$$\mathbf{A}_\infty(\lambda) = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 2\lambda & 0 & 0 \\ -2\lambda & 1 & 0 & 0 \end{bmatrix}. \tag{5.6}$$

By (4.26),

$$\sigma_{\text{ess}}(\mathcal{L}_\infty) = \{\lambda = iy \,|\, y \in (-\infty, -1/2] \cup [1/2, \infty)\}. \tag{5.7}$$

For the rest of this chapter, we assume $\lambda \notin \sigma_{\text{ess}}(\mathcal{L}_\infty)$. For the sech solution, the assumptions of Hypothesis 4.2.2, are satisfied, and so by Theorem 4.2.3 and Proposition 4.2.4, if $\lambda \neq 0$, then $\mathbf{A}_\infty(\lambda)$ has four distinct eigenvalues, $\sigma_\pm = \sqrt{1 \pm 2i\lambda}$ and $-\sigma_\pm = -\sqrt{1 \pm 2i\lambda}$. If $\lambda = 0$, then $\mathbf{A}_\infty(\lambda)$ has 2 eigenvalues, $\pm\sigma = \pm 1$, each of multiplicity 2. We recall that by Proposition 4.2.4, $\mathbf{A} := \mathbf{A}_\infty(\lambda)$ can be diagonalized as $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}$, where the diagonal matrix $\mathbf{D}$ contains the eigenvalues of $\mathbf{A}_\infty$. By Corollary 4.2.5, we see that, in the case that $\lambda \neq 0$,

$$\mathbf{P} = \begin{bmatrix} \frac{-i}{\sqrt{1-2i\lambda}} & \frac{i}{1+2i\lambda} & \frac{-i}{1+2i\lambda} & \frac{i}{\sqrt{1-2i\lambda}} \\ \frac{-1}{\sqrt{1-2i\lambda}} & \frac{-1}{\sqrt{1+2i\lambda}} & \frac{1}{\sqrt{1+2i\lambda}} & \frac{1}{\sqrt{1-2i\lambda}} \\ i & -i & -i & i \\ 1 & 1 & 1 & 1 \end{bmatrix}, \tag{5.8}$$

$$\mathbf{D} = \begin{bmatrix} -\sqrt{1-2i\lambda} & 0 & 0 & 0 \\ 0 & -\sqrt{1+2i\lambda} & 0 & 0 \\ 0 & 0 & \sqrt{1+2i\lambda} & 0 \\ 0 & 0 & 0 & \sqrt{1-2i\lambda} \end{bmatrix} \tag{5.9}$$

$$\mathbf{P}^{-1} = \frac{1}{4}\begin{bmatrix} i\sqrt{1-2i\lambda} & -\sqrt{1-2i\lambda} & -i & 1 \\ -i\sqrt{1+2i\lambda} & -\sqrt{1+2i\lambda} & i & 1 \\ i\sqrt{1+2i\lambda} & \sqrt{1+2i\lambda} & i & 1 \\ -i\sqrt{1-2i\lambda} & \sqrt{1-2i\lambda} & -i & 1 \end{bmatrix}, \tag{5.10}$$

and in the case that $\lambda = 0$,

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{bmatrix}, \tag{5.11}$$

$$\mathbf{D} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{5.12}$$

$$\mathbf{P}^{-1} = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}. \tag{5.13}$$

Without loss of generality, we have assumed in both cases that the diagonal matrix $\mathbf{D}$ is arranged such that the eigenvalues with negative real part are located in the top left block. In the case that $\lambda \neq 0$, we have additionally assumed that $\mathrm{Re}(\sigma_-) \geq \mathrm{Re}(\sigma_+)$, to ensure that the diagonal of $\mathbf{D}$ is given in ascending real part.

With this ordering, the projection onto the stable subspace of $\mathbf{A}_\infty$ is given by $\mathbf{Q} = \mathbf{P}\widehat{\mathbf{Q}}\mathbf{P}^{-1}$, where

$$\widehat{\mathbf{Q}} = \begin{bmatrix} \mathbf{I}_{2\times 2} & \mathbf{0}_{2\times 2} \\ \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 2} \end{bmatrix}. \tag{5.14}$$

In the case where $\lambda = 0$, let κ_- be the real part of the eigenvalue whose real part is negative. Then the Bohl and Lyapunov exponents in Section 4.3 are

$$\varkappa_\pm(\mathbf{Q}) = \lambda_\pm(\mathbf{Q}) = \kappa_- = \varkappa'_\pm(\mathbf{Q}) = \lambda'_\pm(\mathbf{Q}). \tag{5.15}$$

In the case where $\lambda \neq 0$, let $\kappa_{2,-} \leq \kappa_{1,-}$ be the real parts of the eigenvalues whose real parts are negative. Then

$$\varkappa'_\pm(\mathbf{Q}) = \lambda'_\pm(\mathbf{Q}) = \kappa_{2,-} \leq \kappa_{1,-} = \varkappa_\pm(\mathbf{Q}) = \lambda_\pm(\mathbf{Q}). \tag{5.16}$$

Next, we compute the matrix $\mathbf{R}$ in (4.28) and its factors $\mathbf{R}_\ell$ and $\mathbf{R}_r$. By (4.29),

$$\mathbf{M}(x) = \begin{bmatrix} 0 & -\operatorname{sech}^2(x) \\ 3\operatorname{sech}^2(x) & 0 \end{bmatrix}, \tag{5.17}$$

and hence,

$$\mathbf{R}(x) = \begin{bmatrix} 0 & 0 \\ -\mathbf{B}^{-1}\mathbf{M}(x) & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -6\operatorname{sech}^2(x) & 0 & 0 & 0 \\ 0 & -2\operatorname{sech}^2(x) & 0 & 0 \end{bmatrix}. \tag{5.18}$$

Since $\mathbf{M}^*\mathbf{M}$ is diagonal, we have that

$$|\mathbf{M}(x)|^{1/2} = \begin{bmatrix} \sqrt{3}\operatorname{sech}(x) & 0 \\ 0 & \operatorname{sech}(x) \end{bmatrix}, \tag{5.19}$$

and that

$$-\mathbf{B}^{-1}\mathbf{M}(x)|\mathbf{M}(x)|^{-1/2} = \begin{bmatrix} -2\sqrt{3}\operatorname{sech}(x) & 0 \\ 0 & -2\operatorname{sech}(x) \end{bmatrix}. \tag{5.20}$$

Therefore, by our definitions of $\mathbf{R}_r(x)$ and $\mathbf{R}_\ell(x)$ in (4.156) and (4.157),

$$\mathbf{R}_r(x) = \begin{bmatrix} \sqrt{3}\operatorname{sech}(x) & 0 & 0 & 0 \\ 0 & \operatorname{sech}(x) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5.21}$$

and

$$\mathbf{R}_\ell(x) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -2\sqrt{3}\,\mathrm{sech}(x) & 0 & 0 & 0 \\ 0 & -2\,\mathrm{sech}(x) & 0 & 0 \end{bmatrix}. \tag{5.22}$$

Using the explicit formulae for $\mathbf{Q}$, $\mathbf{R}_\ell$, and $\mathbf{R}_r$ we obtained above, we can form the Birman-Schwinger kernel $\mathbf{K}(x, y; \lambda)$ and the corresponding operator $\mathcal{K}(\lambda)$ using (4.163). In Proposition 4.5.1, we showed that, in general, $\mathcal{K}(\lambda)$ is a Hilbert-Schmidt operator, and in Theorem 4.5.5, we derived an upper bound on the Hilbert-Schmidt norm $\|\mathcal{K}(\lambda)\|_{\mathcal{J}_2(L^2(\mathbb{R},\mathbb{C}^4))}$. Furthermore, in Theorem 4.7.1, we established conditions which guarantee that $\mathcal{K}(\lambda)$ is a trace class operator. In the next proposition, we specialize these results to the case of the sech solution of the NLSE. This result will be used later to bolster confidence in our numerical method for approximating the Fredholm determinant.

Proposition 5.1.1. *If $\lambda \notin \sigma_{ess}(\mathcal{L}_\infty)$, then the integral operator $\mathcal{K}(\lambda)$ associated with the sech solution of the NLSE is Hilbert-Schmidt, with*

$$\|\mathcal{K}(\lambda)\|_{\mathcal{J}_2(L^2(\mathbb{R},\mathbb{C}^4))} \leq 32\sqrt{5}\mathrm{cond}(\boldsymbol{P}(\lambda)). \tag{5.23}$$

Furthermore, $\mathcal{K}(\lambda)$ is also trace class.

Proof. The pulse $\Psi(x) = \mathrm{sech}(x)$ decays exponentially; indeed,

$$|\,\mathrm{sech}(x)| = \frac{2}{e^x + e^{-x}} \leq 2e^{-|x|}, \ \forall x \in \mathbb{R}. \tag{5.24}$$

Consequently,

$$\|\mathbf{R}(x)\| \leq \sqrt{40}\,\mathrm{sech}(x) \leq 2\sqrt{40}e^{-|x|}, \ \forall x \in \mathbb{R}. \tag{5.25}$$

That is, $\|\mathbf{R}(x)\| \leq C_R e^{-a|x|}$, where $C_R = 2\sqrt{40}$ and $a = 1$, and $\|\mathbf{R}_r\|$ and $\|\mathbf{R}_\ell\|$ have similar exponential decay. Therefore, by Proposition 4.5.3, $\mathcal{K} \in \mathcal{J}_2(\mathbb{R}, \mathbb{C}^4)$. Furthermore, by

Proposition 4.5.3 and Theorem 4.5.5, the Hilbert-Schmidt norm of $\mathcal{K}$ has an upper bound given by

$$\begin{aligned} \|\mathcal{K}\|^2_{\mathcal{J}_2(L^2(\mathbb{R},\mathbb{C}^4))} &\leq \frac{2C^2(\lambda)}{a^2} &(5.26)\\ &= 2(8\sqrt{40}\text{cond}(\mathbf{P}(\lambda)))^2, &(5.27)\end{aligned}$$

which yields (5.23).

The derivative of $\Psi(x)$ also decays exponentially, since

$$\left|\frac{d}{dx}\Psi(x)\right| = |-\operatorname{sech}(x)\tanh(x)| = \frac{2|e^x - e^{-x}|}{(e^x+e^{-x})^2} \leq 2e^{-|x|},\ \forall x \in \mathbb{R}. \quad (5.28)$$

Claim: $\mathcal{K}$ satisfies both Hypotheses 4.6.3 and 4.6.5. Therefore, the associated operator $\mathcal{K}$ is trace class on $L^2(\mathbb{R},\mathbb{C}^4)$.

Proof of Claim. When $\Psi(x) = \operatorname{sech}(x), |\Psi(x)| > 0\,\forall x \in \mathbb{R}$. Additionally,

$$\begin{aligned} [\epsilon\ \gamma]^T &= [0\ 1]^T \neq 0, &(5.29)\\ [\mu\ \nu]^T &= [0\ 0]^T, &(5.30)\end{aligned}$$

which are not both zero. So, Hypothesis 4.6.3 is satisfied. Hypothesis 4.6.5 is also satisfied, since $[\mu\ \nu]^T = \mathbf{0}$, and hence $\det(\mathbf{M}(\operatorname{sech}(x))) > 0\,\forall x \in \mathbb{R}$. □

With these hypotheses satisfied, and with the exponential decay of Ψ and Ψ_x, by Theorem 4.7.1, we have that $\mathcal{K} \in \mathcal{J}_1(\mathbb{R},\mathbb{C}^4)$.

□

Remark. *As a consequence, by Theorem 2.3.10,* $\exists\Gamma > 0$ *such that*

$$|\det_2(\mathcal{I}+\mathcal{K}(\lambda))| \leq \exp\left\{\Gamma\text{cond}^2(\boldsymbol{P}(\lambda))\right\} \quad (5.31)$$

Since we know that $\mathcal{K}$ is both trace class and Hilbert-Schmidt, we can test the accuracy of our numerical method on both the Fredholm determinant and the 2−modified Fredholm determinant. In order to test the accuracy of the regular Fredholm determinant, we derive an analytical formula for the Evans function, in the special case of the sech solution of the NLSE.

5.2 Evaluating the Evans Function

We recall from Proposition 4.7.2 that for the CQ-CGLE or the NLSE, when the Birman-Schwinger operator $\mathcal{K}$ is trace class, the Fredholm determinant is equal to the Evans function. That is,

$$\det(\mathcal{I} + \mathcal{K}(\lambda)) = E(\lambda). \tag{5.32}$$

Although a general analytic formula for the Evans function does not exist, we can derive a formula for it in the special case of the sech solution of the NLSE. Because it is simpler to do, we will first derive this formula for an alternate form of the linearization of the NLSE. Then we will transform the resulting formula for the Evans function back to the formulation of the linearized NLSE that we use. We recall from Section 4.1, that when we derived the linearization of the CQ-CGLE, we first converted the CQ-CGLE in (4.5) for a complex scalar-valued function Ψ to a system of two equations for the real vector-valued function $\mathbf{\Psi} = [\text{Re}(\Psi)\ \text{Im}(\Psi)]^T$. This leads to the linearized equation given by (4.9) - (4.11). With the alternate formulation, we instead work with the complex vector-valued function $\mathbf{\Phi} = [\Psi\ \overline{\Psi}]^T$. These two formulations are related by $\mathbf{\Psi} = \mathbf{P}\mathbf{\Phi}$ for an invertible matrix $\mathbf{P}$.

5.2.1 An Alternate Formulation

First, we consider the version of the NLSE given by

$$i\partial_t\Phi + (\partial_x^2 - 1)\Phi + |\Phi|^2\Phi = 0. \tag{5.33}$$

Letting $\mathbf{\Phi} = [\Phi\ \overline{\Phi}]$, and linearizing about the solution $\Phi(x) = \sqrt{2}\,\text{sech}(x)$, we arrive at the eigenvalue problem

$$\widehat{\mathcal{L}}\mathbf{p} = \lambda\mathbf{p}, \tag{5.34}$$

with

$$\widehat{\mathcal{L}} = (\partial_x^2 - 1)\boldsymbol{\sigma}_3 + 2\,\text{sech}^2(x)(2\boldsymbol{\sigma}_3 + i\boldsymbol{\sigma}_2), \tag{5.35}$$

where

$$\boldsymbol{\sigma}_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{5.36}$$

$$\text{and} \quad \boldsymbol{\sigma}_2 = i \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{5.37}$$

Multiplying both sides of (5.34) on the left by $\boldsymbol{\sigma}_3$, we obtain the equivalent system

$$(\widetilde{\mathcal{L}} - \lambda \mathbf{I})\mathbf{p} = [(\partial_x^2 - 1)\mathbf{I} - \lambda \boldsymbol{\sigma}_3 + 2\,\mathrm{sech}^2(x)\boldsymbol{\sigma}]\mathbf{p} = 0, \tag{5.38}$$

where

$$\boldsymbol{\sigma} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}. \tag{5.39}$$

The associated unperturbed first-order system is of the form

$$\partial_x \mathbf{Y} = \widetilde{\mathbf{A}}(\lambda)\mathbf{Y}, \ \widetilde{\mathbf{Y}} = [\mathbf{p} \ \partial_x \mathbf{p}]^T, \tag{5.40}$$

with

$$\widetilde{\mathbf{A}}(\lambda) := \begin{bmatrix} \mathbf{0}_{2\times 2} & \mathbf{I}_{2\times 2} \\ \mathbf{I}_{2\times 2} + \lambda \boldsymbol{\sigma}_3 & \mathbf{0}_{2\times 2} \end{bmatrix}. \tag{5.41}$$

For $\lambda \in \mathbb{C}$, we introduce the notation

$$\mu = \sqrt{1-\lambda}, \ \nu = \sqrt{1+\lambda}, \tag{5.42}$$

where $\sqrt{\cdot}$ denotes the principal branch of the square root. Therefore, $\mathrm{Re}(\mu) > 0$ and $\mathrm{Re}(\nu) > 0$, provided that $\lambda \in \mathbb{C} \setminus (-\infty, -1]$ and $\lambda \in \mathbb{C} \setminus [1, \infty)$, respectively. For definiteness, we will often assume that $\mathrm{Re}(\nu) < \mathrm{Re}(\mu)$, but the cases where $\mathrm{Re}(\nu) \geq \mathrm{Re}(\mu)$ would be treated similarly. Using the method of undetermined coefficients, we can conclude that the eigenvalue problem (5.38) has the solutions

$$\mathbf{p} = e^{-\mu x}[(\lambda - 2 - 2\mu \tanh(x))\mathbf{v} + \mathrm{sech}^2(x)\mathbf{w}], \tag{5.43}$$

$$\mathbf{q} = e^{-\nu x}[(-\lambda - 2 - 2\nu \tanh(x))\mathbf{u} + \mathrm{sech}^2(x)\mathbf{w}], \tag{5.44}$$

for

$$\mathbf{u} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \mathbf{v} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \text{ and } \mathbf{w} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \tag{5.45}$$

That is, each of

$$\mathbf{Y}_1 := [\mathbf{p}\ \partial_x \mathbf{p}]^T, \tag{5.46}$$

$$\mathbf{Y}_2 := [\mathbf{q}\ \partial_x \mathbf{q}]^T \tag{5.47}$$

solve the perturbed equation

$$\partial_x \mathbf{Y} = (\widetilde{\mathbf{A}}(\lambda) + \widetilde{\mathbf{R}}(x))\mathbf{Y},\ \mathbf{Y} = [\mathbf{p}\ \partial_x \mathbf{p}]^T, \tag{5.48}$$

where

$$\widetilde{\mathbf{R}}(x) := \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ -2\operatorname{sech}^2(x)\mathbf{I} & \mathbf{0} \end{bmatrix}. \tag{5.49}$$

$$\sigma(\widetilde{\mathbf{A}}(\lambda)) = \{-\mu, -\nu, \nu, \mu\} \tag{5.50}$$

are precisely the eigenvalues of $\widetilde{\mathbf{A}}$ in (5.41), with corresponding eigenvectors

$$\mathbf{y}_1 := \begin{bmatrix} \mathbf{v} \\ -\mu\mathbf{v} \end{bmatrix},\ \mathbf{y}_2 := \begin{bmatrix} \mathbf{u} \\ -\nu\mathbf{u} \end{bmatrix},\ \mathbf{y}_3 := \begin{bmatrix} \mathbf{u} \\ \nu\mathbf{u} \end{bmatrix},\ \text{and } \mathbf{y}_4 := \begin{bmatrix} \mathbf{v} \\ \mu\mathbf{v} \end{bmatrix}. \tag{5.51}$$

The projections $\mathbf{Q}_1$ onto Span$\{\mathbf{y}_1\}$ parallel to Span$\{\mathbf{y}_2, \mathbf{y}_3, \mathbf{y}_4\}$, $\mathbf{Q}_2$ onto Span$\{\mathbf{y}_2\}$ parallel to Span$\{\mathbf{y}_1, \mathbf{y}_3, \mathbf{y}_4\}$, $\mathbf{Q}_3$ onto Span$\{\mathbf{y}_3\}$ parallel to Span$\{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_4\}$, and $\mathbf{Q}_4$ onto Span$\{\mathbf{y}_4\}$

parallel to $\mathrm{Span}\{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3\}$ are given by

$$\mathbf{Q}_1 := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & -\frac{1}{2\mu} \\ 0 & 0 & 0 & 0 \\ 0 & -\frac{\mu}{2} & 0 & \frac{1}{2} \end{bmatrix}, \tag{5.52}$$

$$\mathbf{Q}_2 := \begin{bmatrix} \frac{1}{2} & 0 & -\frac{1}{2\nu} & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{\nu}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5.53}$$

$$\mathbf{Q}_3 := \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2\nu} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{\nu}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{5.54}$$

$$\text{and } \mathbf{Q}_4 := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2\mu} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{\mu}{2} & 0 & \frac{1}{2} \end{bmatrix}, \tag{5.55}$$

respectively.

We can verify directly that the fundamental matrix solution $\mathbf{\Phi}$ of the unperturbed problem $\mathbf{\Phi}' = \widetilde{\mathbf{A}}(\lambda)\mathbf{\Phi}$ is given by

$$\mathbf{\Phi}(x) := \begin{bmatrix} \cosh(\nu x) & 0 & \frac{1}{\nu}\sinh(\nu x) & 0 \\ 0 & \cosh(\mu x) & 0 & \frac{1}{\mu}\sinh(\mu x) \\ \nu\sinh(\nu x) & 0 & \cosh(\nu x) & 0 \\ 0 & \mu\sinh(\mu x) & 0 & \cosh(\mu x) \end{bmatrix}. \tag{5.56}$$

The Bohl and Lyapunov exponents are

$$\varkappa(\mathbf{Q}_1) = -\operatorname{Re}(\mu),\ \varkappa(\mathbf{Q}_2) = -\operatorname{Re}(\nu),\ \varkappa(\mathbf{Q}_3) = \operatorname{Re}(\nu), \text{ and } \varkappa(\mathbf{Q}_4) = \operatorname{Re}(\mu). \tag{5.57}$$

Additionally,

$$\mathbf{\Phi}(x)\mathbf{Q}_1 = \begin{bmatrix} 0 & e^{-\mu x}\widehat{\mathbf{w}}_2 & 0 & e^{-\mu x}\widehat{\mathbf{w}}_4 \end{bmatrix},\ \widehat{\mathbf{w}}_2 := \begin{bmatrix} \frac{1}{2}\mathbf{v} \\ -\frac{\mu}{2}\mathbf{v} \end{bmatrix},\ \widehat{\mathbf{w}}_4 := \begin{bmatrix} -\frac{1}{2\mu}\mathbf{v} \\ \frac{1}{2}\mathbf{v} \end{bmatrix}, \tag{5.58}$$

$$\mathbf{\Phi}(x)\mathbf{Q}_2 = \begin{bmatrix} e^{-\nu x}\widehat{\mathbf{w}}_1 & 0 & e^{-\nu x}\widehat{\mathbf{w}}_3 & 0 \end{bmatrix},\ \widehat{\mathbf{w}}_1 := \begin{bmatrix} \frac{1}{2}\mathbf{u} \\ -\frac{\nu}{2}\mathbf{u} \end{bmatrix},\ \widehat{\mathbf{w}}_4 := \begin{bmatrix} -\frac{1}{2\nu}\mathbf{u} \\ \frac{1}{2}\mathbf{u} \end{bmatrix}. \tag{5.59}$$

Without loss of generality, assume that $\operatorname{Re}(\nu) < \operatorname{Re}(\mu)$. The generalized matrix Jost solutions which solve the perturbed problem as defined in [20, Definition 7.2] are those 4×4 matrix-valued solutions $\mathbf{Y}_+^{(j)}, j = 1, 2$, and $\mathbf{Y}_-^{(j)}, j = 3, 4$, which satisfy the conditions

$$\limsup_{x\to\infty} \frac{1}{x} \ln \|\mathbf{Y}_+^{(j)} - \mathbf{\Phi}(x)\mathbf{Q}_j\| < \varkappa(\mathbf{Q}_j),\ j = 1, 2, \tag{5.60}$$

$$\liminf_{x\to-\infty} \frac{1}{x} \ln \|\mathbf{Y}_-^{(j)} - \mathbf{\Phi}(x)\mathbf{Q}_j\| > \varkappa(\mathbf{Q}_j),\ j = 3, 4. \tag{5.61}$$

If we define

$$\mathbf{Y}_+(x) := \mathbf{Y}_+^{(1)}(x) + \mathbf{Y}_+^{(2)}(x), \tag{5.62}$$

$$\mathbf{Y}_-(x) := \mathbf{Y}_-^{(3)}(x) + \mathbf{Y}_-^{(4)}(x), \tag{5.63}$$

$$\text{and } \mathbf{Y}(x) := \mathbf{Y}_+(x) + \mathbf{Y}_-(x), \tag{5.64}$$

then the Evans determinant is given by

$$\widetilde{E} = \det(\mathbf{Y}(0)). \tag{5.65}$$

In order to calculate the components of $\mathbf{Y}$, we first find solutions $\mathbf{Y}_+^{(1)}$ and $\mathbf{Y}_+^{(2)}$, such that

$$e^{\operatorname{Re}(\mu)x} \left\| \mathbf{Y}_+^{(1)}(x) - \mathbf{\Phi}(x)\mathbf{Q}_1 \right\| = O(1) \text{ as } x \to \infty, \tag{5.66}$$

$$e^{\operatorname{Re}(\nu)x} \left\| \mathbf{Y}_+^{(2)}(x) - \mathbf{\Phi}(x)\mathbf{Q}_2 \right\| = O(1) \text{ as } x \to \infty. \tag{5.67}$$

Let $\mathbf{z}_k^{(j)}, k = 1,2,3,4$, denote the columns of the matrix $\mathbf{Y}_+^{(j)}(x)$, $j = 1,2$. To satisfy (5.66), (5.67), we need to find complex constants $a_k^{(j)}$ and $b_k^{(j)}$ such that

$$e^{\mathrm{Re}(\mu)x}\left\| a_k^{(1)}\begin{bmatrix}\mathbf{q}\\ \mathbf{q}_x\end{bmatrix} + b_k^{(1)}\begin{bmatrix}\mathbf{p}\\ \mathbf{p}_x\end{bmatrix} - \mathbf{w}_k^{(1)}\right\| = O(1) \text{ as } x\to\infty, \tag{5.68}$$

$$e^{\mathrm{Re}(\nu)x}\left\| a_k^{(2)}\begin{bmatrix}\mathbf{q}\\ \mathbf{q}_x\end{bmatrix} + b_k^{(2)}\begin{bmatrix}\mathbf{p}\\ \mathbf{p}_x\end{bmatrix} - \mathbf{w}_k^{(2)}\right\| = O(1) \text{ as } x\to\infty, \tag{5.69}$$

where $\mathbf{p}$ and $\mathbf{q}$ are the solutions (5.43) and (5.44), and $\mathbf{w}_k^{(j)}$ are the columns of the matrix $\mathbf{\Phi}(x)\mathbf{Q}_j$ from (5.58) and (5.59). Then

$$\mathbf{z}_k^{(j)} = a_k^{(j)}\begin{bmatrix}\mathbf{p}_2\\ \partial_x\mathbf{p}_2\end{bmatrix} + b_k^{(j)}\begin{bmatrix}\mathbf{p}_1\\ \partial_x\mathbf{p}_1\end{bmatrix}, \tag{5.70}$$

and

$$\mathbf{Y}_+(x) = \begin{bmatrix}\mathbf{z}_1^{(1)}+\mathbf{z}_1^{(2)} & \mathbf{z}_2^{(1)}+\mathbf{z}_2^{(2)} & \mathbf{z}_3^{(1)}+\mathbf{z}_3^{(2)} & \mathbf{z}_4^{(1)}+\mathbf{z}_4^{(2)}\end{bmatrix}. \tag{5.71}$$

Lemma 5.2.1. *Assuming that* $\mathrm{Re}(\nu) < \mathrm{Re}(\mu)$, *the constants*

$$a_1 := \frac{1}{2(-\lambda-2-2\nu)},\ b_2 := \frac{1}{2(\lambda-2-2\mu)},\ a_3 := -\frac{a_1}{\nu},\ \textit{and } b_4 := -\frac{b_2}{\mu} \tag{5.72}$$

satisfy the conditions (5.68) and (5.69). Then

$$\boldsymbol{Y}_+^{(1)}(x) = \begin{bmatrix}0 & b_2\begin{bmatrix}\boldsymbol{p}\\ \boldsymbol{p}_x\end{bmatrix} & 0 & b_4\begin{bmatrix}\boldsymbol{p}\\ \boldsymbol{p}_x\end{bmatrix}\end{bmatrix}, \tag{5.73}$$

$$\boldsymbol{Y}_+^{(2)}(x) = \begin{bmatrix}a_1\begin{bmatrix}\boldsymbol{q}\\ \boldsymbol{q}_x\end{bmatrix} & 0 & a_3\begin{bmatrix}\boldsymbol{q}\\ \boldsymbol{q}_x\end{bmatrix} & 0\end{bmatrix}, \tag{5.74}$$

$$\textit{and } \boldsymbol{Y}_+(x) = \begin{bmatrix}a_1\begin{bmatrix}\boldsymbol{q}\\ \boldsymbol{q}_x\end{bmatrix} & b_2\begin{bmatrix}\boldsymbol{p}\\ \boldsymbol{p}_x\end{bmatrix} & a_3\begin{bmatrix}\boldsymbol{q}\\ \boldsymbol{q}_x\end{bmatrix} & b_4\begin{bmatrix}\boldsymbol{p}\\ \boldsymbol{p}_x\end{bmatrix}\end{bmatrix}. \tag{5.75}$$

Furthermore,

$$\boldsymbol{Y}_-(x) = \widehat{\boldsymbol{\sigma}}_3\,\boldsymbol{Y}_+(-x)\widehat{\boldsymbol{\sigma}}_3, \tag{5.76}$$

where

$$\widehat{\boldsymbol{\sigma}}_3 \;:=\; \begin{bmatrix} \boldsymbol{I}_{2\times 2} & \boldsymbol{0} \\ \boldsymbol{0} & -\boldsymbol{I}_{2\times 2} \end{bmatrix}. \tag{5.77}$$

Proof. Consider formulas (5.43) and (5.44) written in the form

$$\mathbf{p} \;= e^{-\mu x}\big(f\cdot v + h\big),\ \mathbf{p}' = e^{-\mu x}\big(-\mu f\cdot v + h\big), \tag{5.78}$$

$$\mathbf{q} \;= e^{-\nu x}\big(g\cdot u + h\big),\ \mathbf{q}' = e^{-\nu x}\big(-\nu g\cdot u + h\big), \tag{5.79}$$

where we define

$$f(x) := \lambda - 2 - 2\mu\tanh(x) \;\;\to\;\; \lambda - 2 - 2\mu = -(1+\mu)^2 \text{ as } x\to\infty, \tag{5.80}$$

$$g(x) := -\lambda - 2 - 2\nu\tanh(x) \;\;\to\;\; -\lambda - 2 - 2\nu = -(1+\nu)^2 \text{ as } x\to\infty, \tag{5.81}$$

and denote by h a generic function such that $h(x), h'(x) = O(1)$ as $x\to\infty$. Recall that $\mathbf{w}_1^{(1)} = 0$ by (5.58), and $e^{\mathrm{Re}(\mu)-\mathrm{Re}(\nu)} \to \infty$ as $x\to\infty$, by assumption. Thus, by (5.68), when $k = 1$, it must be that both $a_1^{(1)}$ and $b_1^{(1)}$ are zero. For $k = 2$, by (5.68), $a_2^{(1)} = 0$, and by (5.58), $\mathbf{w}_1 = e^{-\mu x}\widehat{\mathbf{w}}_1$. This gives that $b_2^{(1)} = b_2$, for b_2 defined in (5.72). An analogous argument shows that $a_3^{(1)} = a_r^{(1)} = b_3^{(1)} = 0$ and $b_4^{(1)} = b_4$, where b_4 is defined in (5.72). This gives the desire result for $\mathbf{Y}_+^{(1)}$. The argument for $a_k^{(2)}$ and $b_k^{(1)}$, and thus for $\mathbf{Y}_+^{(2)}$, is similar.

Now that we have a formula for $\mathbf{Y}_+$, we must develop one for $\mathbf{Y}_-$, using the cases $j = 3, 4$. Using (5.73) and (5.74), we define

$$\mathbf{Y}_-^{(3)}(x) \;:=\; \widehat{\boldsymbol{\sigma}}_3\mathbf{Y}_+^{(2)}(-x)\widehat{\boldsymbol{\sigma}}_3, \tag{5.82}$$

$$\text{and } \mathbf{Y}_-^{(4)}(x) \;:=\; \widehat{\boldsymbol{\sigma}}_3\mathbf{Y}_+^{(1)}(-x)\widehat{\boldsymbol{\sigma}}_3, \tag{5.83}$$

for $\widehat{\boldsymbol{\sigma}}_3$ defined in (5.77). Since $\widetilde{\mathbf{R}}(x)$ in (5.49) is even, and since $\mathbf{Y}_+^{(j-2)}$ is a solution of (5.48), a direct computation shows that $\mathbf{Y}_-^{(j)}$ solves (5.48) for $j = 3, 4$. To show that $\mathbf{Y}_-^{(j)}$, $j = 3, 4$

satisfies (5.61), we notice that $\widehat{\boldsymbol{\sigma}}_3$ is unitary and that $\widehat{\boldsymbol{\sigma}}_3\mathbf{Q}_3\widehat{\boldsymbol{\sigma}}_3 = \mathbf{Q}_2$, and so, using (5.57) and replacing x by $-x$, we calculate that

$$\begin{aligned}
\liminf_{x\to-\infty} \ln \left\|\mathbf{Y}_-^{(3)}(x) - \mathbf{\Phi}(x)\mathbf{Q}_3\right\| &= \liminf_{x\to-\infty} \frac{1}{x} \ln \left\|\widehat{\boldsymbol{\sigma}}_3\mathbf{Y}_-^{(2)}(-x)\widehat{\boldsymbol{\sigma}}_3 - \mathbf{\Phi}(x)\mathbf{Q}_3\right\| && (5.84)\\
&= -\limsup_{x\to\infty} \frac{1}{x} \ln \left\|\widehat{\boldsymbol{\sigma}}_3(\mathbf{Y}_+^{(2)} - \mathbf{\Phi}(x)\mathbf{Q}_2)\widehat{\boldsymbol{\sigma}}_3\right\| && (5.85)\\
&= -\limsup_{x\to\infty} \frac{1}{x} \ln \left\|\mathbf{Y}_+^{(2)} - \mathbf{\Phi}(x)\mathbf{Q}_2\right\| && (5.86)\\
&> -\varkappa(\mathbf{Q}_2) && (5.87)\\
&= \varkappa(\mathbf{Q}_3), && (5.88)
\end{aligned}$$

as required. The argument for $j = 4$ is analogous. It follows that

$$\mathbf{Y}(x) = \mathbf{Y}_+(x) + \widehat{\boldsymbol{\sigma}}_3\mathbf{Y}_-(-x)\widehat{\boldsymbol{\sigma}}_3 \tag{5.89}$$

can be represented as the block matrix

$$\mathbf{Y}(x)=\begin{bmatrix} a_1(\mathbf{q}(x)+\mathbf{q}(-x)) & b_2(\mathbf{p}(x)+\mathbf{p}(-x)) & a_3(\mathbf{q}(x)-\mathbf{q}(-x)) & b_4(\mathbf{p}(x)-\mathbf{p}(-x)) \\ a_1(\mathbf{q}'(x)-\mathbf{q}'(-x)) & b_2(\mathbf{p}'(x)-\mathbf{p}'(-x)) & a_3(\mathbf{q}'(x)+\mathbf{q}'(-x)) & b_4(\mathbf{p}'(x)+\mathbf{p}'(-x)) \end{bmatrix}.$$

□

Then, by (5.64) and (5.65), we find that

$$\begin{aligned}
\widetilde{E}(\lambda) = \det(\mathbf{Y}(0)) &= \det[2a_1\mathbf{q}(0)\, 2b_2\mathbf{p}(0)] \times \det[2a_3\mathbf{q}'(0)\, 2b_4\mathbf{p}'(0)] && (5.90)\\
&= 16\lambda^4 a_1 b_2 a_3 b_4 \mu\nu && (5.91)\\
&= \frac{\lambda^4}{(1+\mu)^4(1+\nu)^4}. && (5.92)
\end{aligned}$$

We can use this result to define the Evans function for our formulation of the NLSE using a change of variables and a similarity transform.

Proposition 5.2.2. *Let $\boldsymbol{v}$ be a solution of the eigenvalue problem $\widetilde{\mathcal{L}}\boldsymbol{v} = \widetilde{\lambda}\boldsymbol{v}$ for $\widetilde{\mathcal{L}}$ as defined in (5.38), where $\boldsymbol{Y} = [\boldsymbol{v}\,\boldsymbol{v}_x]^T$ solves*

$$\partial_x \boldsymbol{Y} = (\widetilde{\boldsymbol{A}}(\widetilde{\lambda}) + \widetilde{\boldsymbol{R}}(x)), \tag{5.93}$$

for $\widetilde{\boldsymbol{A}}$ *and* $\widetilde{\boldsymbol{R}}(x)$ *as defined in (5.41) and (5.49), respectively. Define the matrix*

$$\boldsymbol{P} := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}. \tag{5.94}$$

Then the vector $\boldsymbol{u} = \boldsymbol{P}\boldsymbol{v}$ *is a solution of the eigenvalue problem* $\mathcal{L}\boldsymbol{u} = \lambda\boldsymbol{u}$*, for* $\mathcal{L}$ *as defined in (4.10), with eigenvalue* $\lambda = \frac{i}{2}\widetilde{\lambda}$*, and* $\boldsymbol{Z} = [\boldsymbol{u}\,\boldsymbol{u}_x]^T$ *solves the equation*

$$\partial_x \boldsymbol{Z} = (\boldsymbol{A}(\lambda) + \boldsymbol{R}(x))\boldsymbol{Z}, \tag{5.95}$$

where $\boldsymbol{A}$ *and* $\boldsymbol{R}$ *are defined in (4.24) and (4.134), respectively. Consequently, the Evans function which determines the spectrum of* $\mathcal{L}$ *can be given by*

$$E(\lambda) = -\widetilde{E}(-2i\lambda), \tag{5.96}$$

with $\widetilde{E}$ *as defined in (5.90).*

Proof. First, we note that

$$\mathbf{P}\mathbf{P}^* = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix} \begin{bmatrix} 1 & i \\ 1 & -i \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} = \mathbf{I}_{2\times 2}. \tag{5.97}$$

Assume that

$$(\widetilde{\mathcal{L}} - \widetilde{\lambda}\mathbf{I})\mathbf{v} = [(\partial_x^2 - 1)\mathbf{I} - \widetilde{\lambda}\boldsymbol{\sigma}_3 + 2\,\mathrm{sech}^2(x)\boldsymbol{\sigma}]\mathbf{v} = 0. \tag{5.98}$$

Note that $(\mathcal{L} - \lambda)\mathbf{u} = 0 \iff (2\mathcal{L} - 2\lambda)\mathbf{u} = 0$. Considering the latter eigenvalue equation, for $\mathcal{L}$ as defined in (4.10), and letting $\mathbf{u} = \mathbf{P}\mathbf{v}$, we have that

$$\left[(\partial_x^2 - 1)\mathbf{J} - 2\lambda\mathbf{I} + 2\,\mathrm{sech}^2(x) \begin{bmatrix} 0 & -1 \\ 3 & 0 \end{bmatrix} \right] \mathbf{P}\mathbf{v} = 0, \tag{5.99}$$

where

$$\mathbf{J} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{5.100}$$

Multiplying by $\mathbf{P}^*$ on the left, where $\mathbf{P}^*\mathbf{P} = \mathbf{I}$, we have that

$$\left[(\mathbf{P}^*\mathbf{J}\mathbf{P})(\partial_x^2 - 1) - 2\lambda\mathbf{I} + 2\,\mathrm{sech}^2(x)\mathbf{P}^* \begin{bmatrix} 0 & -1 \\ 3 & 0 \end{bmatrix} \mathbf{P}\right] \mathbf{v} = 0. \tag{5.101}$$

Now,

$$\mathbf{P}^*\mathbf{J}\mathbf{P} = \mathbf{K}, \tag{5.102}$$

where

$$\mathbf{K} := \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \tag{5.103}$$

and

$$\mathbf{P}^* \begin{bmatrix} 0 & -1 \\ 3 & 0 \end{bmatrix} \mathbf{P} = 2i\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_2. \tag{5.104}$$

So (5.101) holds when

$$[(\partial_x^2 - 1)\mathbf{K} - 2\lambda + 2\,\mathrm{sech}^2(x)(2i\boldsymbol{\sigma}_3 - \boldsymbol{\sigma}_2)]\mathbf{v} = 0. \tag{5.105}$$

Multiplying on the left by $i\boldsymbol{\sigma}_3$, and noting that $-(i\boldsymbol{\sigma}_3)^2 = \mathbf{I}$, we obtain the equivalent problem

$$[(\partial_x^2 - 1) + 2i\lambda\boldsymbol{\sigma}_3 + 2\,\mathrm{sech}^2(x)(2\mathbf{I} + i\boldsymbol{\sigma}_3\boldsymbol{\sigma}_2)]\mathbf{v} = 0, \tag{5.106}$$

which is precisely the equation

$$(\widetilde{\mathcal{L}} + 2i\lambda)\mathbf{v} = 0, \tag{5.107}$$

so that $(\mathcal{L} - \lambda)\mathbf{u} = 0$ and $(\widetilde{\mathcal{L}} - (-2i\lambda))\mathbf{v} = 0$ are equivalent. The vector $\mathbf{Y} = [\mathbf{v}\,\mathbf{v}_x]^T$ solves

$$\partial_x\mathbf{Y} = (\widetilde{\mathbf{A}}(\lambda) + \widetilde{\mathbf{R}}(x))\mathbf{Y}, \tag{5.108}$$

and so $\mathbf{Z} = \widetilde{\mathbf{P}}\mathbf{Y} = [\mathbf{u}\,\mathbf{u}_x]^T$ solves the transformed problem

$$\partial_x\mathbf{Z} = \widetilde{\mathbf{P}}[\widetilde{\mathbf{A}}(-2i\lambda) + \widetilde{\mathbf{R}}(x)]\widetilde{\mathbf{P}}^*\mathbf{Z}. \tag{5.109}$$

Therefore, the solutions $\mathbf{Y}_+(x), \mathbf{Y}_-(x)$ in (5.75) and (5.76) are computed by replacing λ with $-2i\lambda$, and the corresponding Jost solutions are $\mathbf{Z}_\pm = \widetilde{\mathbf{P}}\mathbf{Y}_\pm$. Defining $\mathbf{Z} := \mathbf{Z}_+ + \mathbf{Z}_-$, we have that

$$\begin{aligned} E(\lambda) &= \det(\mathbf{Z}(0)) && (5.110)\\ &= \det\left(\widetilde{\mathbf{P}}\mathbf{Y}(0)\right) && (5.111)\\ &= \det\left(\widetilde{\mathbf{P}}\right)\det(\mathbf{Y}(0)) && (5.112)\\ &= -\widetilde{E}(-2i\lambda), && (5.113) \end{aligned}$$

since

$$\det\left(\widetilde{\mathbf{P}}\right) = (\det(\mathbf{P}))^2 = -1. \tag{5.114}$$

□

We will use this Evans function to test the accuracy of our numerically computed regular Fredholm determinant.

Remark. *From numerical simulations, we found that there is a global minus sign error in the computation of either the Evans function or the Fredholm determinant. We have not yet found the source of this sign discrepancy. This does not affect any results on the magnitude of the determinant or on the ability to calculate roots of the determinant, but for the purpose of evaluating the relative error between the Evans function and the determinant, in the following simulations, we will redefine*

$$E(\lambda) := \frac{16\lambda^4}{(1+\mu(\lambda))^4(1+\nu(\lambda))^4}, \tag{5.115}$$

where

$$\mu(\lambda) := \sqrt{1-2i\lambda},\ \nu(\lambda) := \sqrt{1+2i\lambda}. \tag{5.116}$$

5.3 Numerical Approximation of the Fredholm Determinant

We recall that when we estimate the Fredholm determinant, we first truncate $\mathcal{K}$ from $\mathbb{R}$ to a finite interval $[-L, L]$, for some $0 < L < \infty$, as outlined in Section 2.4. We estimate the truncation error to be

$$\left|\det_p(\mathcal{I} + \mathcal{K}) - \det_p(\mathcal{I} + \mathcal{K}|_{[-L,L]})\right| \leq e^{-aL}\mathbf{\Phi}\left(\frac{8C}{a}\right), \tag{5.117}$$

for both $p = 1$ and 2. Here, the constants C and a are such that $|K_{ij}(x, y)| \leq Ce^{-a(|x|+|y|)}$ $i, j \in \{1, \ldots, 4\}$, $\forall x, y$. We know that these constants exists as $\Psi(x) = \text{sech}(x)$ decays exponentially. We then apply the composite Simpson's rule to evaluate the truncated integrals within the Fredholm determinant. The associated quadrature error can be bounded, as in Section 2.5, by

$$\left|\det_p(\mathcal{I} + \mathcal{K}|_{[-L,L]}) - \det_{p,Q}(\mathcal{I} + \mathcal{K}|_{[-L,L]})\right| \leq \frac{\sqrt{2\pi}e}{8}\Delta x\mathbf{\Phi}(8L\|\mathbf{K}\|_{W^{1,\infty}}), \tag{5.118}$$

where Δx is the spacing in the quadrature rule.

Next, we present figures from a numerical simulation where we evaluate the regular and $2-$modified Fredholm determinants for $\Psi(x) = \text{sech}(x)$.

5.3.1 Truncation and Quadrature Errors

We evaluate the soliton pulse $\Psi(x) = \text{sech}(x)$ and test our error bounds. We know that, by Proposition 5.2.2, $\lambda = 0$ is a zero of $\det_p(\mathcal{I} + \mathcal{K}(\lambda))$, for $p = 1$ and 2, so we study the numerical error for this value of λ. In Figure 5.1, we evaluate the error between $\det_2(\mathcal{I}+\mathcal{K}(0))$ and its approximation, for varied interval widths L, for a constant spacing $\Delta x = 0.0293$. We see an exponential decay in the error as L increases from 1 to about 2.8, and, as expected, we see that for sufficiently large L, the error is dominated by the quadrature error, dictated by the spacing Δx.

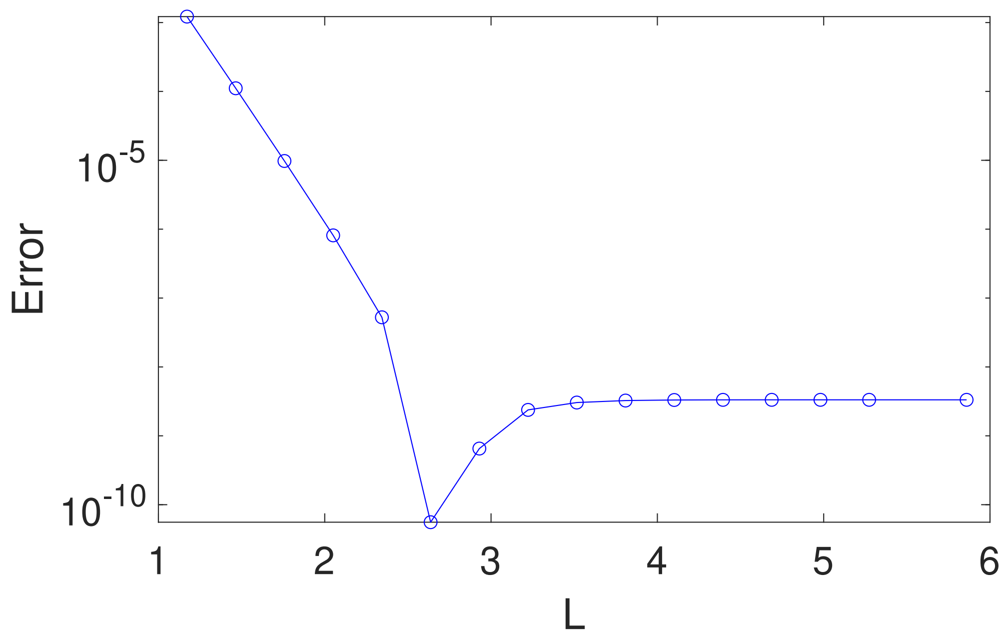

Figure 5.1. The error between the numerically computed $\det_{1,Q}(\mathcal{I} + \mathcal{K}(0))$ and the true determinant.

In Figure 5.2, we plot the numerical error in computing $\det_2(\mathcal{I}+\mathcal{K}(0))$ for several values of Δx, using an interval of width $L \approx 7.32$, which by Figure 5.2 we know to be sufficiently large. We know from Theorem 4.8.1 that for fixed L, the quadrature error should behave, at worst, as $O(\Delta x)$, but in this figure we see that the true numerical error behaves as $O(\Delta x^4)$, the maximum level of accuracy achievable by the composite Simpson's rule. If we consider Proposition 5.4.1 in the appendix to this chapter, we see that in the sech case, $\mathbf{K}$ is C^∞ almost everywhere, so it is not surprising that we get a higher order of accuracy than that which results from being only Lipschitz continuous.

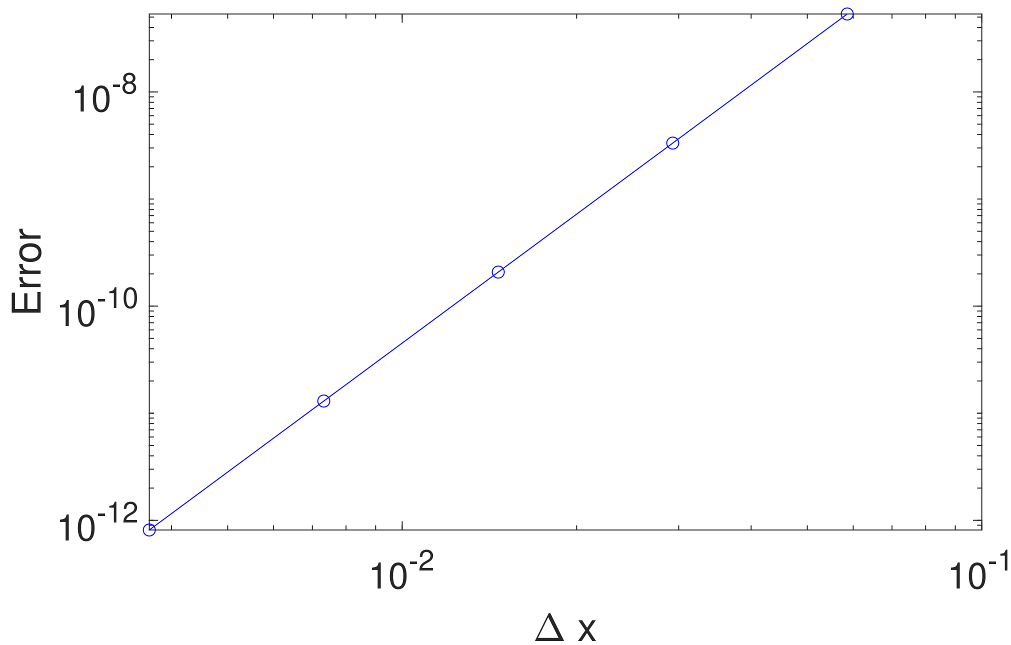

Figure 5.2. We observe the error between $|\det_{1,Q}(\mathcal{I} + \mathcal{K}(0))|$ and the true determinant, for various values of Δx.

In particular, we see that using a spacing of $\Delta x \approx 0.0037$, the error between $\det_{2,Q}(\mathcal{I} + \mathcal{K}(0))$ and the true 2−modified determinant, 0, is less than 10^{-12}.

In Figure 5.3, we can see further evidence of the error's dependence upon Δx by examining the behavior of the Fredholm determinant, for several values of Δx, plotted as functions of λ as $\lambda \to 0$. We compare to the Evans function along the same line and show that the numerical determinant gains approximately one order of magnitude in accuracy each time Δx is halved, for values of λ approaching the eigenvalue zero of $\mathcal{L}$.

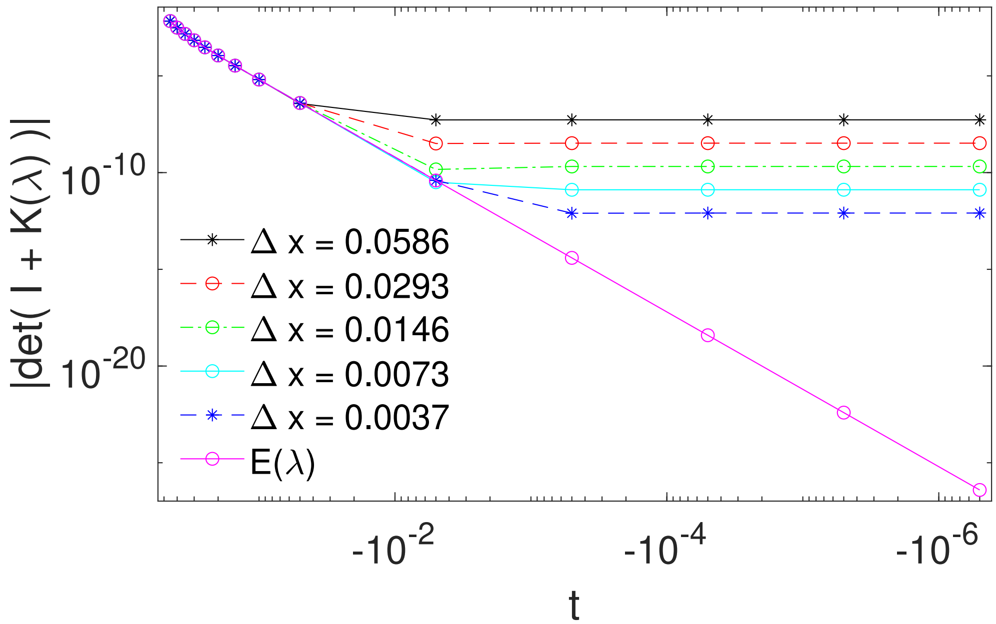

Figure 5.3. Dependence of the approximated determinant $|\det_{1,Q}(\mathcal{I}+\mathcal{K}(\lambda))|$ on the quadrature spacing Δx, as $\lambda \to 0$ along the line $\lambda(t) = it$.

5.3.2 Error in Determinant Calculations for a Known Eigenvalue

We continue to study the behavior of our numerically approximated determinants near the known eigenvalue $\lambda = 0$. Because the error using the spacing $\Delta x = 0.0037$ yields a sufficiently small error in computing this root ($|\text{Error}| \leq 10^{-12}$), we will continue to use this spacing. In Figures 5.4. 5.5, and 5.6, we plot the regular and 2−modified Fredholm determinant for values of λ approaching 0 along the real axis, the imaginary axis, and along a line through the complex plane, respectively. We can plot both the Fredholm determinant and 2−modified Fredholm determinant on the same axes, since at $\lambda = 0$, the ratio between these determinants is $O(1)$.

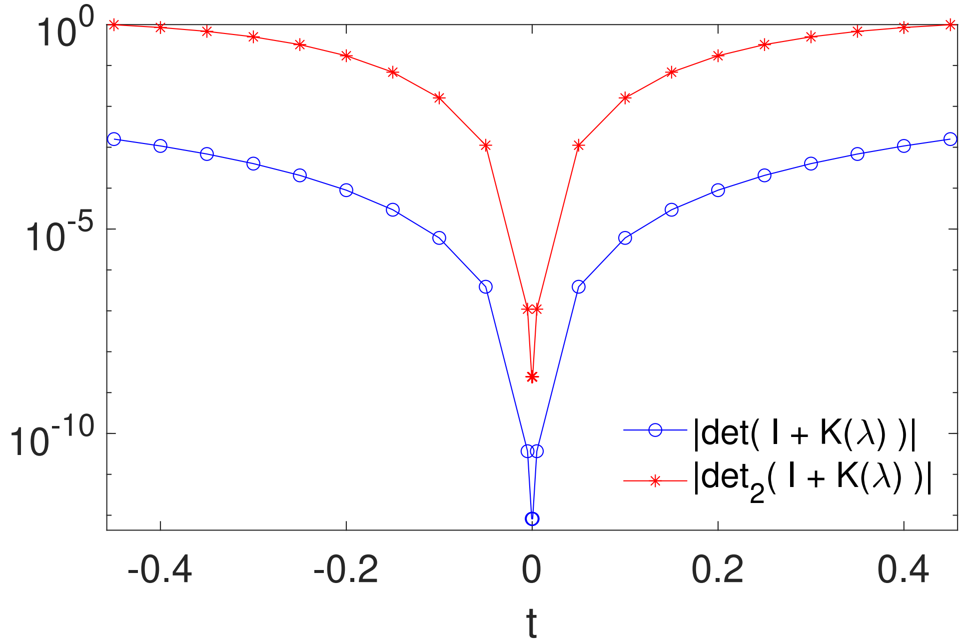

Figure 5.4. Plot of $|\det_p(\mathcal{I}+\mathcal{K}(\lambda))|$, for $p=1$ and 2, along the line $\lambda(t)=t$.

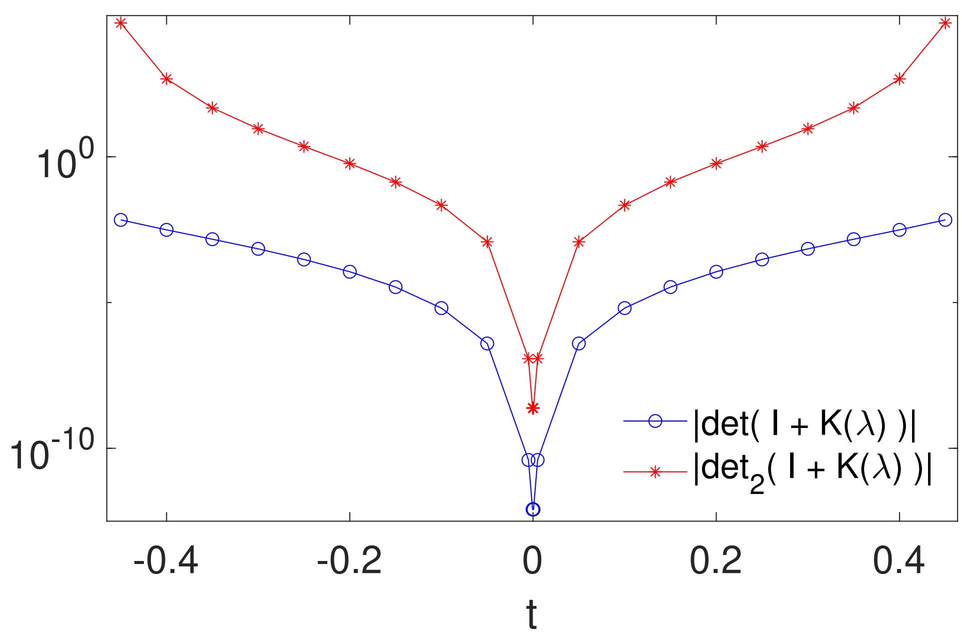

Figure 5.5. Plot of $|\det_p(\mathcal{I}+\mathcal{K}(\lambda))|$, for $p=1$ and 2, along the line $\lambda(t)=it$.

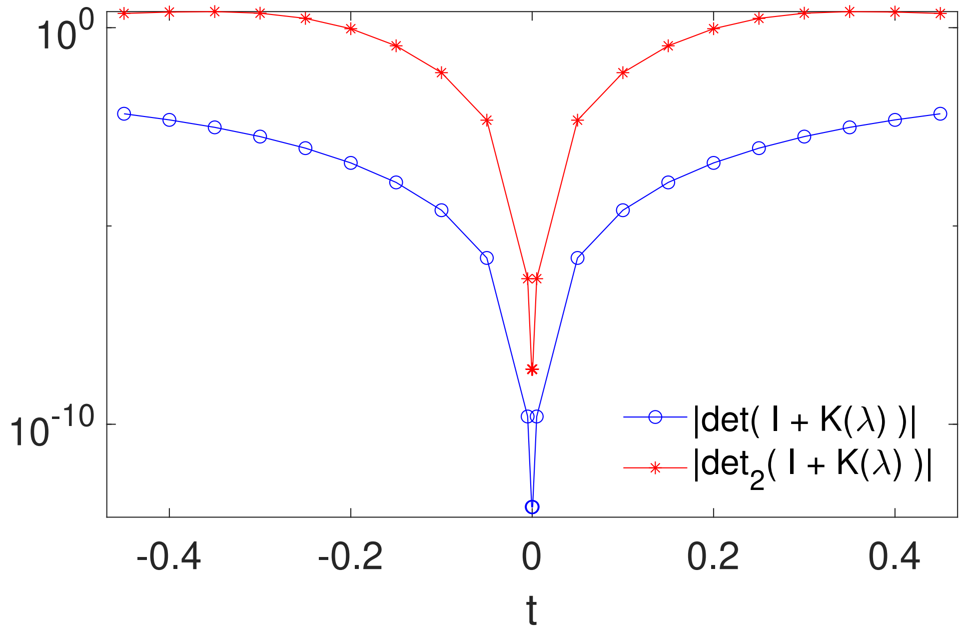

Figure 5.6. Plot of $|\det_p(\mathcal{I}+\mathcal{K}(\lambda))|$, for $p=1$ and 2, along the line $\lambda(t)=(1-i)t$.

5.3.3 Error and Behavior Near the Essential Spectrum

We now consider the behavior of $\det_p(\mathcal{I}+\mathcal{K}(\lambda))$, for $p=1$ and 2, for values of λ near $\sigma_{\text{ess}}(\mathcal{L}_\infty)$, as this will be where the determinant is most poorly behaved, and additionally, where the numerical error will be highest, due to the format of $\mathbf{P}$ as described in (5.8).

For $\mathcal{L}_\infty$ with $\Psi(x)=\text{sech}(x)$, the essential spectrum is given by

$$\sigma_{\text{ess}}(\mathcal{L}_\infty)=\{\lambda\in i\mathbb{R}|\lambda=|\lambda|\geq 1/2\}. \tag{5.119}$$

We study the behavior of the Fredholm determinants as we approach the edge of the essential spectrum, evaluated on the interval $[-7.32, 7.32]$.

In Figure 5.7, we plot $\det_{1,Q}(\mathcal{I}+\mathcal{K}(\lambda))$ for various values of Δx, as λ approaches the edge of the essential spectrum at $\lambda=0.5i$ along the imaginary axis, and we compare these results to the Evans function. We note that the numerically computed regular Fredholm determinant behaves erratically as we get sufficiently close to the edge, but that this effect decreases as Δx decreases. In particular, for $\Delta x \approx 0.0037$, the numerical determinant behaves sufficiently like the Evans function.

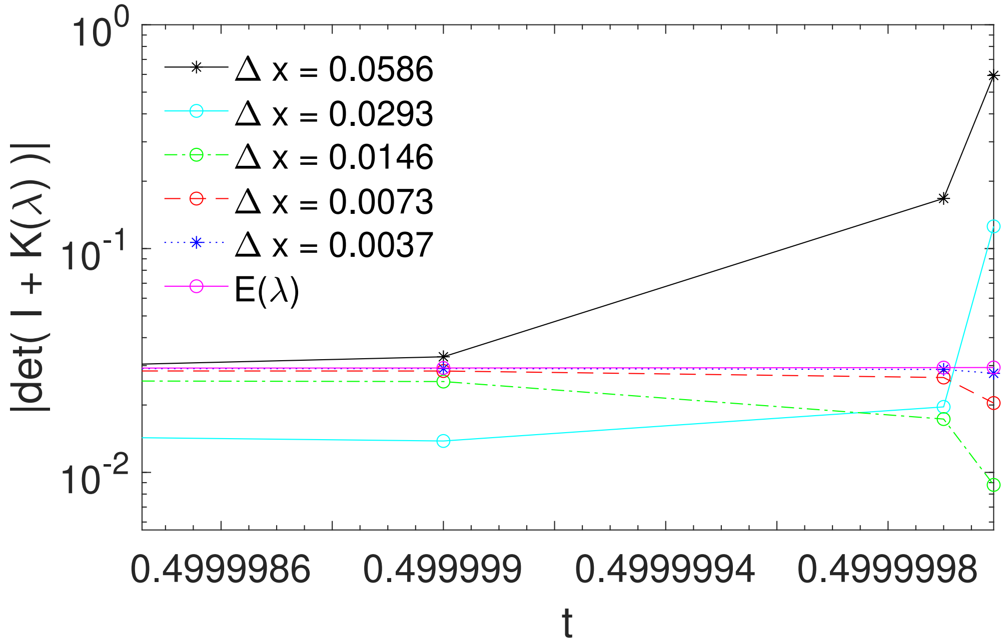

Figure 5.7. $|\det(\mathcal{I} + \mathcal{K}(\lambda))|$ as $\lambda \to 0.5i$ along the imaginary axis, for various values of Δx.

Therefore, in the following plots, we use a truncated interval of $[-7.32, 7.32]$ and a quadrature spacing of $\Delta x \approx 0.0037$ to study the Fredholm determinant as λ approaches the essential spectrum.

In Figure 5.8, we evaluate the Fredholm determinant as λ approaches $\lambda = 0.5i$ along the imaginary axis. As expected, the determinant gets larger as we approach the edge of the essential spectrum, but since $\mathcal{K}$ is trace class, we know the determinant is finite for all $\lambda \notin \sigma_{\text{ess}}(\mathcal{L})$.

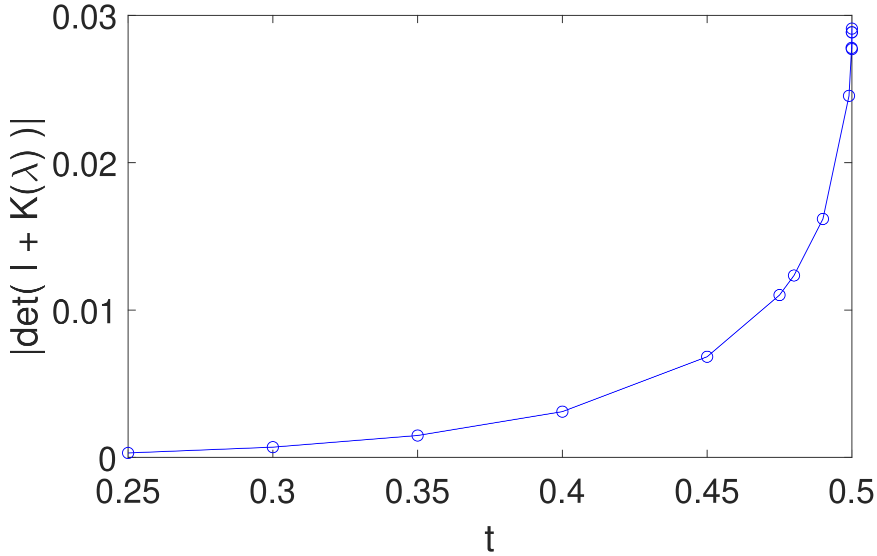

Figure 5.8. We model the behavior of $|\det_{1,Q}(\mathcal{I} + \mathcal{K}(\lambda))|$ for $\lambda(t) = it$, as $t \to 0.5$.

In Figure 5.9, we evaluate the Fredholm determinant as λ approaches $\lambda = 0.5i$ along a line parallel to the real axis. We see that as $\lambda \to 0.5i$, the Fredholm determinant appears to approach an approximate value of 0.03 in magnitude, which agrees with the results in Figure 5.8.

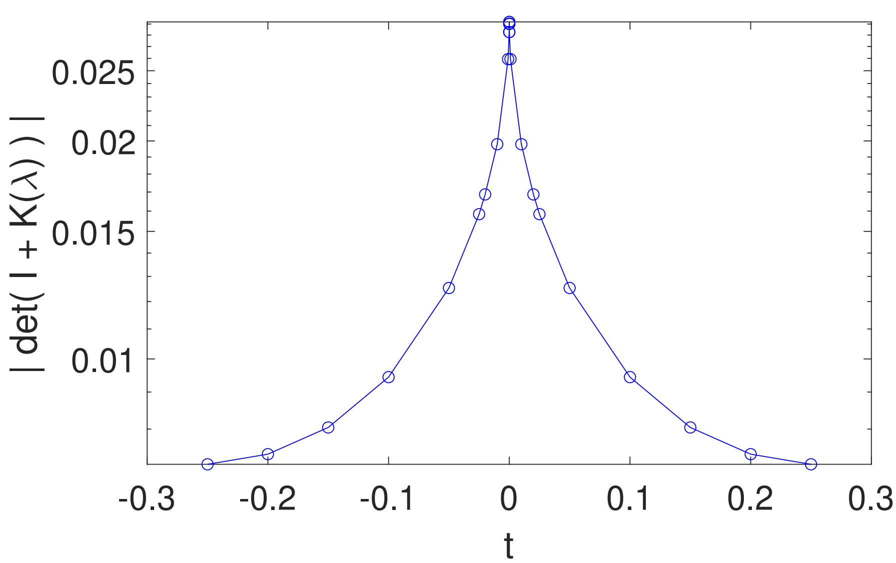

Figure 5.9. Plot of $|\det_{1,Q}(\mathcal{I} + \mathcal{K}(\lambda))|$ for $\lambda(t) = t + 0.5i$.

In Figure 5.10, we evaluate the Fredholm determinant as λ approaches $\lambda = 0.5i$ through the complex plane. The approximate value of $|\det(\mathcal{I} + \mathcal{K}(0.5i))|$ agrees with the previous simulations as $\lambda \to 0.5i$ from different directions.

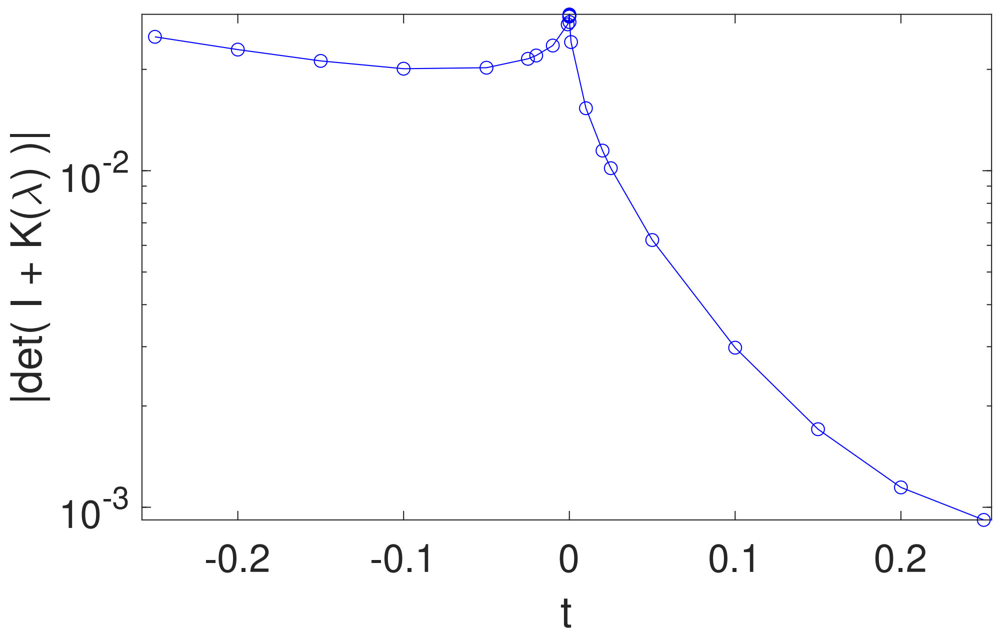

Figure 5.10. Plot of $|\det_{1,Q}(\mathcal{I}+\mathcal{K}(\lambda))|$ for $\lambda(t) = (1-i)t+0.5i$. The value $t = 0$ corresponds to $\lambda = 0.5i$

The regular Fredholm determinant appears to behave relatively well, even near the edge of the essential spectrum. Because we know the Evans function for this particular example, we can compare the behavior of the determinant to the Evans function. Next, we will show that our numerically approximated Fredholm determinant agrees with the Evans function, except when very close to the edge of the essential spectrum.

In Figures 5.11, 5.12, and 5.13, we plot the relative error between the numerically approximated Fredholm determinant and the Evans function for values of λ approaching the edge of the essential spectrum, along the lines $\lambda(t) = it$, $\lambda(t) = t + 0.5i$, and $\lambda(t) = (1-i)t + 0.5i$, respectively. In all three cases, we notice a significant increase in the relative error as we approach $\lambda = 0.5i$. Nevertheless, the relative error here is of $O(10^{-2})$, which suggests great accuracy in our numerical approximation. Undoubtedly, for an even smaller quadrature spacing, the relative error would decrease even more.

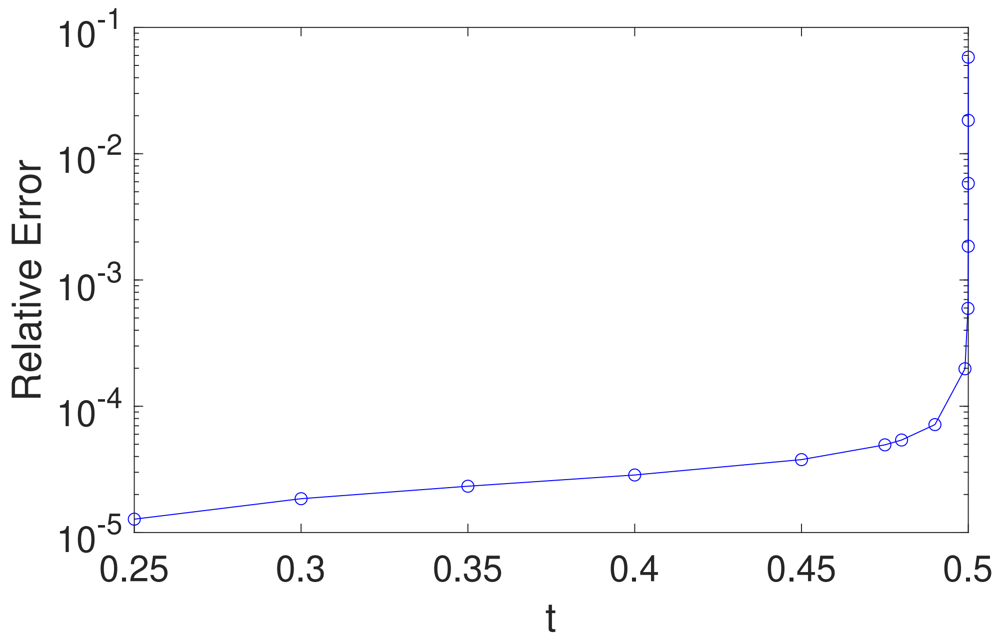

Figure 5.11. Relative Error between $\det_{1,Q}(\mathcal{I} + \mathcal{K}(\lambda))$ and $E(\lambda)$ as $\lambda \to 0.5i$ along the line $\lambda(t) = it$.

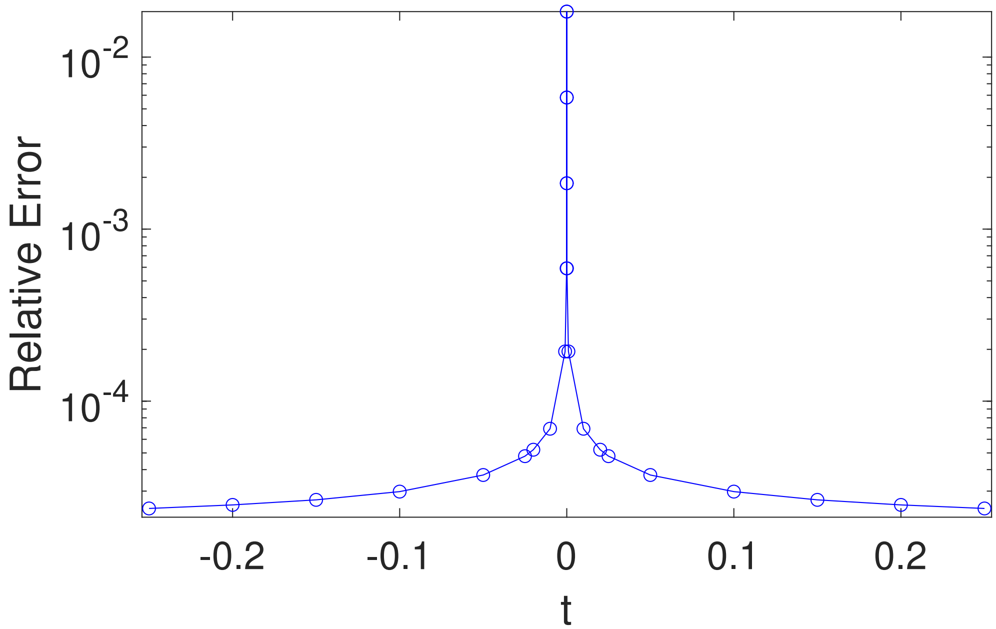

Figure 5.12. Relative Error between $\det_{1,Q}(\mathcal{I} + \mathcal{K}(\lambda))$ and $E(\lambda)$ as $\lambda \to 0.5i$ along the line $\lambda(t) = t + 0.5i$.

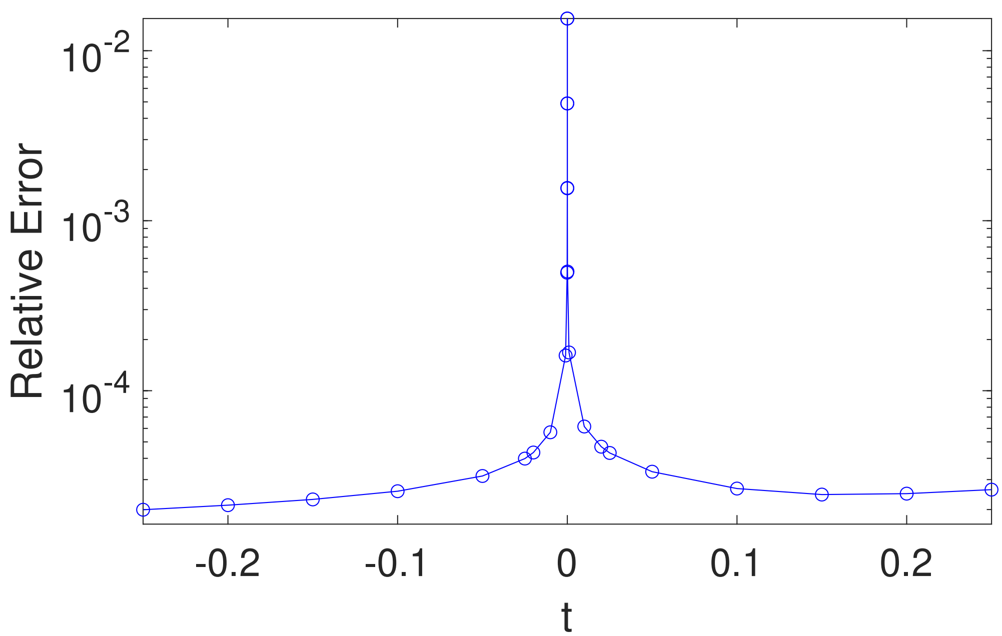

Figure 5.13. Relative Error between $\det_{1,Q}(\mathcal{I} + \mathcal{K}(\lambda))$ and $E(\lambda)$ as $\lambda \to 0.5i$ along the line $\lambda(t) = (1 - i)t + 0.5i$.

Because we know $\mathcal{K}$ is a trace class operator away from the essential spectrum, it is necessarily also Hilbert-Schmidt. In Figure 5.14, we look at the behavior of the 2−modified Fredholm determinant as λ approaches the essential spectrum along the imaginary axis. Since $\mathcal{K} \in \mathcal{J}_2$, the 2−modified determinant should be bounded for all λ, but from Theorem 4.5.5, we know that this bound is λ−dependent.

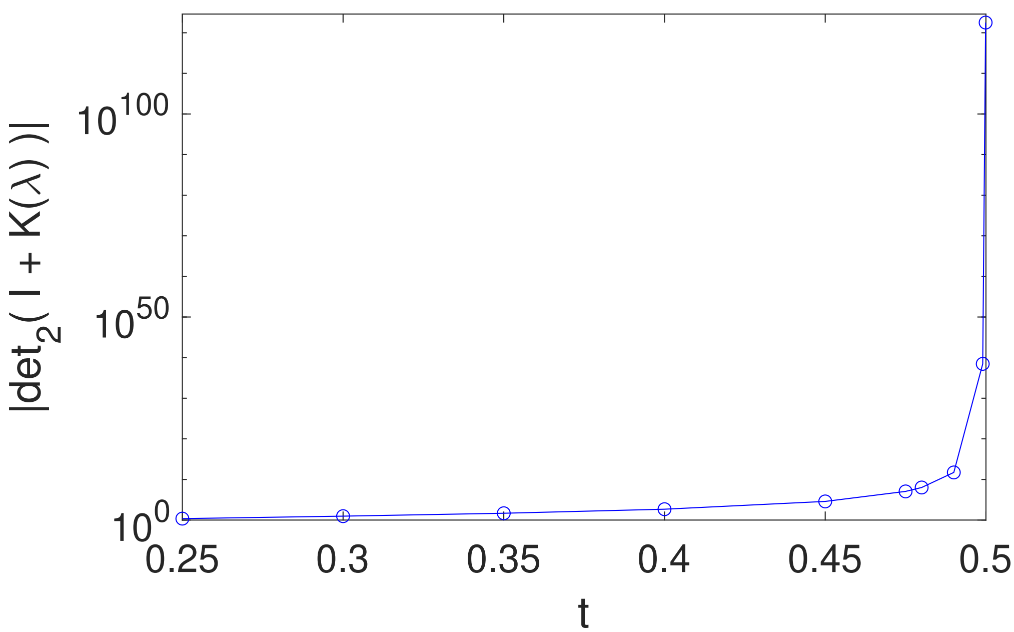

Figure 5.14. Plot of $|\det_{2,Q}(\mathcal{I} + \mathcal{K}(\lambda))|$ as $\lambda(t) = it$ approaches $\sigma_{\text{ess}}(\mathcal{L}_\infty)$.

We see that the 2−modified Fredholm determinant of $\mathcal{K}(\lambda)$ appears to blow up as λ approaches the essential spectrum along the line $\lambda(t) = it$. The behavior of the 2−modified determinant near the essential spectrum is therefore extremely different from the regular Fredholm determinant. The determinant appears to tend to infinity in norm as λ converges to the edge of the essential spectrum. This behavior is due to the determinant's dependence on the condition number of the matrix $\mathbf{P}(\lambda)$, as demonstrated in Theorem 4.5.5.

We expect to see similar behavior as λ approaches the edge $\lambda = 0.5i$ of $\sigma_{\text{ess}}(\mathcal{L})$ along any line. In Figure 5.15, we observe a similar blowup in the 2−modified determinant for λ approaching the essential spectrum along the line $\lambda(t) = 0.5i + t$, and in Figure 5.16, we see even worse behavior at the edge of the essential spectrum along the line $\lambda(t) = (1-i)t + 0.5i$.

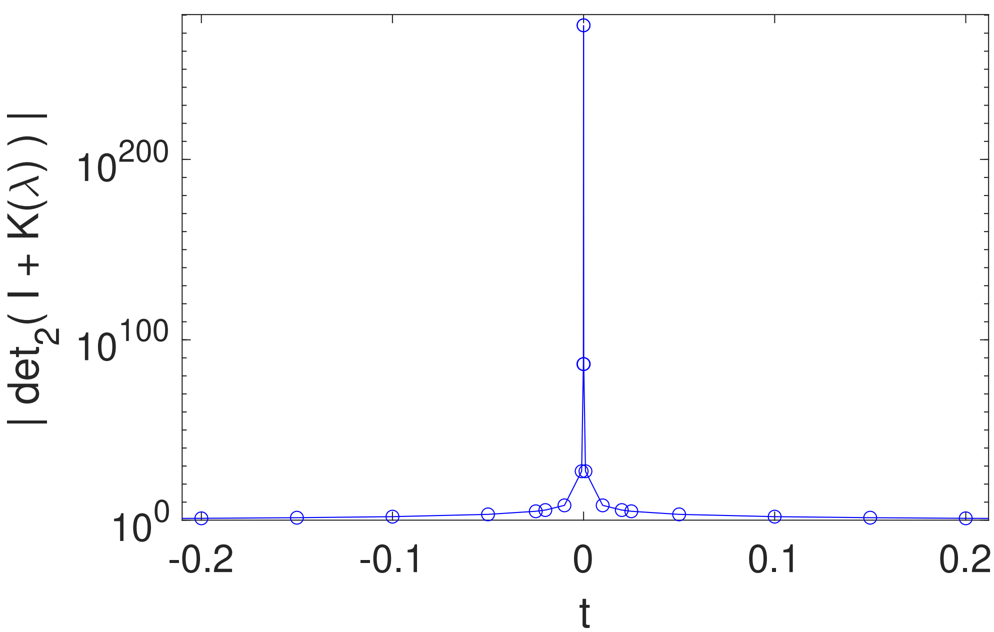

Figure 5.15. Plot of $|\det_{2,Q}(\mathcal{I} + \mathcal{K}(\lambda))|$ as $\lambda(t) = 0.5i + t$ approaches the edge of the essential spectrum.

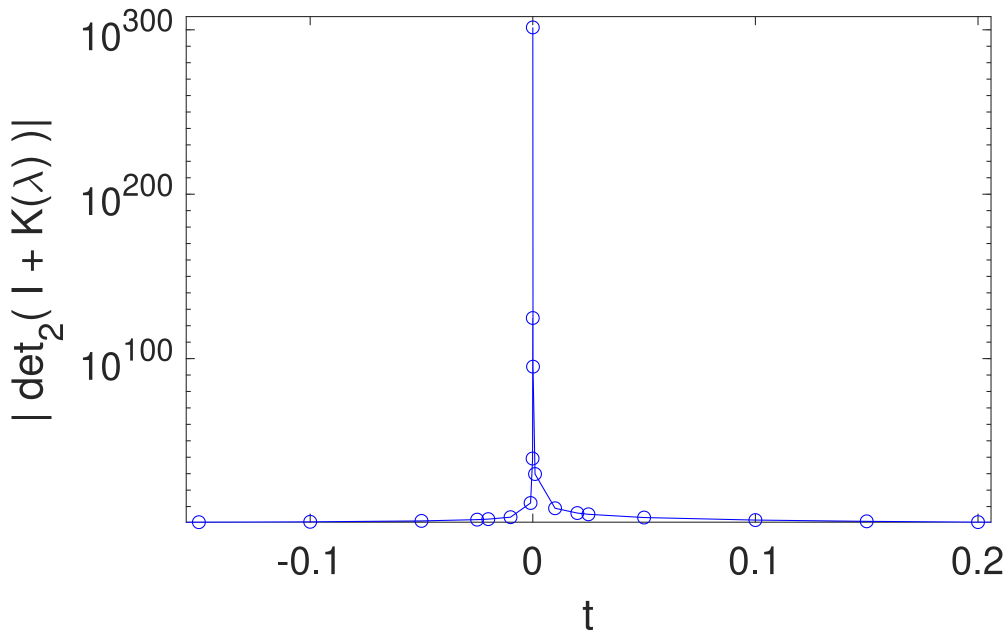

Figure 5.16. Plot of $|\det_{2,Q}(\mathcal{I} + \mathcal{K}(\lambda))|$, as λ approaches $\sigma_{\text{ess}}(\mathcal{L}_\infty)$ along the line $\lambda(t) = (1-i)t + 0.5i$.

By (5.31), we know that the behavior of the 2−modified Fredholm determinant is due to its exponential dependence on the condition number of the matrix $\mathbf{P}(\lambda)$. Since

$$c_1 \|\mathbf{P}\|_{\max} \|\mathbf{P}^{-1}\|_{\max} \leq \text{cond}(\mathbf{P}(\lambda)) \leq c_2 \|\mathbf{P}\|_{\max} \|\mathbf{P}^{-1}\|_{\max}, \tag{5.120}$$

and since when $\lambda \to \sigma_{\text{ess}}(\mathcal{L})$, either $\mu \to 0$, or $\nu \to 0$, causing $\|\mathbf{P}\|_{\max} \to \infty$, we expect $\text{cond}(\mathbf{P}(\lambda))$ to have poles at both edges of the essential spectrum.

In Figure 5.17, we can see that (5.31) is, in fact, an upper bound on $|\det_2(\mathcal{I}+\mathcal{K}(\lambda))|$, as we model it for $\lambda(t) = it$ as $t \to 0.5$. We see further confirmation in Figures 5.18 and 5.19, that in fact,

$$|\det_2(\mathcal{I} + \mathcal{K}(\lambda))| \leq |\exp\{\text{cond}^2(\mathbf{P}(\lambda))\}|. \tag{5.121}$$

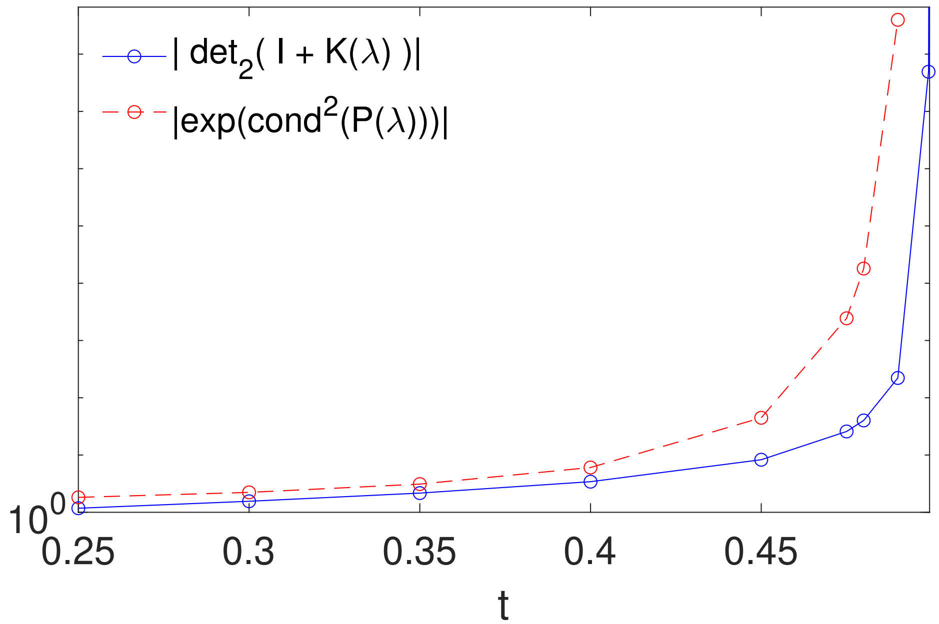

Figure 5.17. Validation of the estimate $|\det_{2,Q}(\mathcal{I} + \mathcal{K}(\lambda))| \leq |\exp\big(\text{cond}^2(\mathbf{P}(\lambda))\big)|$, along the line $\lambda(t) = it$.

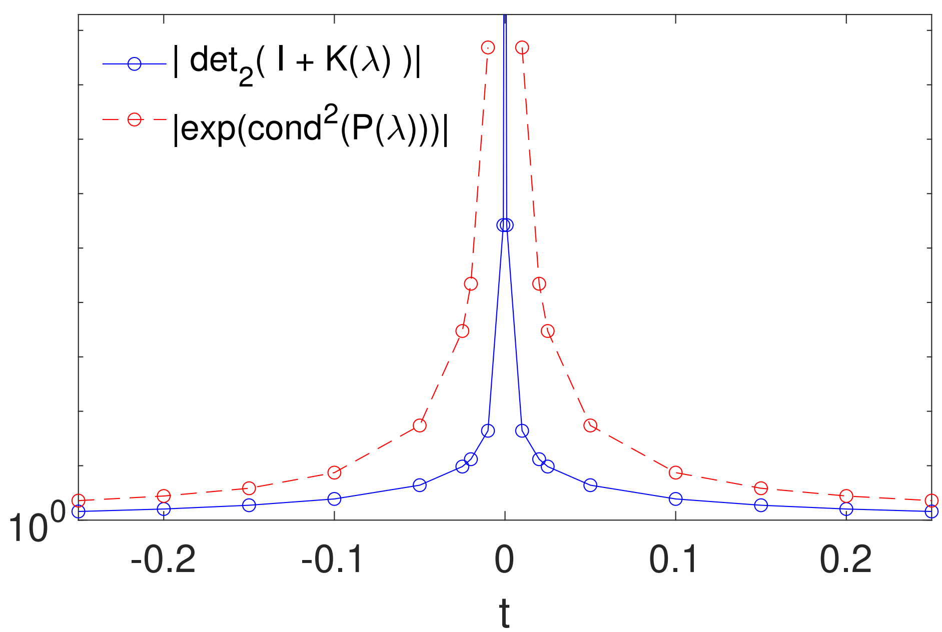

Figure 5.18. Validation of the estimate $|\det_{2,Q}(\mathcal{I} + \mathcal{K}(\lambda))| \leq |\exp\big(\text{cond}^2(\mathbf{P}(\lambda))\big)|$, along the line $\lambda(t) = t + 0.5i$.

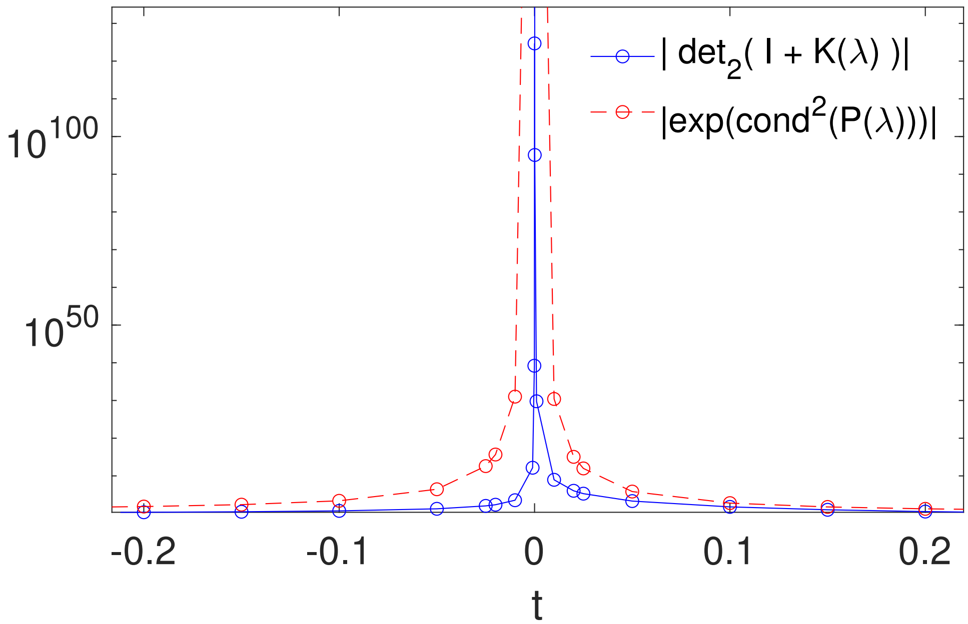

Figure 5.19. Validation of the estimate $|\det_{2,Q}(\mathcal{I}+\mathcal{K}(\lambda))| \leq |\exp\big(\text{cond}^2(\mathbf{P}(\lambda))\big)|$, along the line $\lambda(t) = (1-i)t + 0.5i$.

We see that the regular and $2-$modified Fredholm determinants of $\mathcal{K}(\lambda)$ are indeed bounded for each λ. However, we have seen that in the case of the sech solution, the $2-$modified Fredholm determinant of $\mathcal{K}$ behaves as though it has poles at the edges of $\sigma_{\text{ess}}(\mathcal{L})$, while the regular Fredholm determinant does not. This behavior is to be expected, because $\det_2(\mathcal{I}+\mathcal{K}) = e^{-\operatorname{Tr}(\mathcal{K})}\det_1(\mathcal{I}+\mathcal{K})$, and as we show in the next result, in the sech case, $\operatorname{Re}(\operatorname{Tr}(\mathcal{K})) < 0$, where $\operatorname{Tr}(\mathcal{K})$ has poles at the edges of $\sigma_{\text{ess}}(\mathcal{L})$.

Proposition 5.3.1. *For the solution* $\Psi(x) = \operatorname{sech}(x)$ *of the NLSE, the quantity in (4.271) is given by*

$$\Theta = 4\left[\sqrt{\frac{1}{1+2i\lambda}} + \sqrt{\frac{1}{1-2i\lambda}}\right], \tag{5.122}$$

where $\sqrt{\cdot}$ *denotes the principal square root. In particular,* $|\Theta| \to \infty$ *as* $\lambda \to \pm i/2$*. Additionally, since by Proposition 4.7.2,* $\operatorname{Tr}(\mathcal{K}) = -\Theta$*, this means that*

$$\operatorname{Re}(\operatorname{Tr}(\mathcal{K})) < 0, \tag{5.123}$$

and so $|\det_2(\mathcal{I}+\mathcal{K}(\lambda))| \geq |\det_1(\mathcal{I}+\mathcal{K}(\lambda))|$.

Proof. We recall that $\mathrm{Tr}(\mathcal{K}) = \int_{\mathbb{R}} \mathrm{Tr}(\mathbf{K}(x,x))dx$, where $\mathbf{K}$ is given by

$$\mathbf{K}(x,x') = \begin{cases} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}(x-x')}\mathbf{R}_\ell(x'), & x \geq x', \\ \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}(x-x')}\mathbf{R}_\ell(x'), & x < x'. \end{cases} \tag{5.124}$$

This gives that, for fixed λ,

$$\mathbf{K}(x,x;\lambda) = -\mathbf{R}_r(x)\mathbf{Q}(\lambda)\mathbf{R}_\ell(x). \tag{5.125}$$

We express the projection, $\mathbf{Q}$, onto the stable subspace of $\mathbf{A}_\infty$,

$$\mathbf{Q} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \\ \mathbf{Q}_3 & \mathbf{Q}_4 \end{bmatrix}. \tag{5.126}$$

Since $\mathbf{A}_\infty(\lambda) = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}$, by (4.84), $\mathbf{Q}$ is of the form $\mathbf{Q} = \mathbf{P}\widehat{\mathbf{Q}}\mathbf{P}^{-1}$. Recall that the perturbation operator, $\mathbf{R}(x)$, is given by

$$\mathbf{R}(x) = \begin{bmatrix} \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 2} \\ -\mathbf{B}^{-1}\mathbf{M}(x) & \mathbf{0}_{2\times 2} \end{bmatrix} = \begin{bmatrix} \mathbf{0}_{2\times 2} & \mathbf{0}_{2\times 2} \\ \widetilde{\mathbf{R}} & \mathbf{0}_{2\times 2} \end{bmatrix}. \tag{5.127}$$

Then following (5.21) and (5.22), we find that

$$\begin{aligned} \mathbf{K}(x,x) &= \begin{bmatrix} -\sqrt{3}\,\mathrm{sech}(x) & 0 & 0 & 0 \\ 0 & -\mathrm{sech}(x) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & Q_{14} \\ Q_{21} & Q_{22} & Q_{23} & Q_{24} \\ Q_{31} & Q_{32} & Q_{33} & Q_{34} \\ Q_{41} & Q_{42} & Q_{43} & Q_{44} \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -2\sqrt{3}\,\mathrm{sech}(x) & 0 & 0 & 0 \\ 0 & -2\,\mathrm{sech}(x) & 0 & 0 \end{bmatrix} \\ &= \mathrm{sech}^2(x) \begin{bmatrix} 6Q_{13} & 2\sqrt{3}Q_{14} & 0 & 0 \\ 2\sqrt{3}Q_{23} & 2Q_{24} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \end{aligned} \tag{5.128}$$

In the case that $\lambda \neq 0$,

$$\mathbf{K}(x,x;\lambda) = \frac{\operatorname{sech}^2(x)}{2}\begin{bmatrix} -3\left[\frac{1}{\sqrt{1-2i\lambda}} + \frac{1}{\sqrt{1+2i\lambda}}\right] & \sqrt{3}i\left[\frac{1}{\sqrt{1+2i\lambda}} - \frac{1}{\sqrt{1-2i\lambda}}\right] & 0 & 0 \\ -\sqrt{3}i\left[\frac{1}{\sqrt{1+2i\lambda}} - \frac{1}{\sqrt{1-2i\lambda}}\right] & -\left[\frac{1}{\sqrt{1-2i\lambda}} + \frac{1}{\sqrt{1+2i\lambda}}\right] & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad (5.129)$$

and so

$$\operatorname{Tr}(\mathbf{K}(x,x)) = -2\operatorname{sech}^2(x)\left[\frac{1}{\sqrt{1-2i\lambda}} + \frac{1}{\sqrt{1+2i\lambda}}\right]. \quad (5.130)$$

Similarly, in the case that $\lambda = 0$,

$$\mathbf{K}(x,x;0) = \operatorname{sech}^2(x)\begin{bmatrix} -3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad (5.131)$$

and so

$$\operatorname{Tr}(\mathbf{K}(x,x;0)) = -4\operatorname{sech}^2(x). \quad (5.132)$$

We compute that

$$\int_{-\infty}^{\infty}\operatorname{sech}^2(x)dx = \lim_{y\to\infty}\tanh(y) - \lim_{y\to-\infty}\tanh(y) = 2. \quad (5.133)$$

and so, when $\lambda \neq 0$,

$$\operatorname{Tr}(\mathcal{K}(\lambda)) = -4\left[\frac{1}{\sqrt{1-2i\lambda}} + \frac{1}{\sqrt{1+2i\lambda}}\right], \quad (5.134)$$

and when $\lambda = 0$,

$$\operatorname{Tr}(\mathcal{K}(\lambda = 0)) = -8. \quad (5.135)$$

These two formulas for $\operatorname{Tr}(\mathcal{K})$ are consistent, since

$$\lim_{\lambda\to 0} -4\left[\frac{1}{\sqrt{1-2i\lambda}} + \frac{1}{\sqrt{1+2i\lambda}}\right] = -8. \quad (5.136)$$

Since $\Theta = -\operatorname{Tr}(\mathcal{K})$, (5.122) follows. Additionally, $\operatorname{Re}(\operatorname{Tr}(\mathcal{K}(\lambda))) < 0$, and since $\det_2(\mathcal{I}+\mathcal{K}) = e^{-\operatorname{Tr}(\mathcal{K})} \det_1(\mathcal{I}+\mathcal{K})$, we have that

$$|\det_2(\mathcal{I}+\mathcal{K})| \geq |\det_1(\mathcal{I}+\mathcal{K})|. \tag{5.137}$$

Moreover, we see in (5.134) that $\operatorname{Tr}(\mathcal{K})$ has a pole at both edges of the essential spectrum. □

In summary, this result explains and quantifies the blowup of the 2−modified Fredholm determinant as $\lambda \to 0.5i$.

Our numerical simulations confirm our theoretical results that $\mathcal{K}$ is, indeed, both Hilbert-Schmidt and trace class. On the truncated interval $[-7.32, 7.32]$ and using the quadrature spacing $\Delta x \approx 0.0037$, we compute the eigenvalue $0 = \lambda \in \sigma_{\mathrm{pt}}(\mathcal{L})$ within an error of less than 10^{-12}. We show that even where the Fredholm determinant is largest, near the edge of the essential spectrum, we still maintain a low relative error between the true and numerically computed determinants. We conclude that even though $\mathcal{K}$ is both $\mathcal{J}_1$ and $\mathcal{J}_2$, when finding the values λ in the point spectrum of $\mathcal{L}$, we should use the regular Fredholm determinant, rather than the 2−modified determinant, since $\operatorname{Re}(\operatorname{Tr}(\mathcal{K})) < 0$ and hence the 2−modified determinant is always exponentially larger in magnitude than the regular determinant, which will be challenging for either root-finding or contour integral methods for numerically computing zeros of the Fredholm determinant.

5.4 Chapter 5 Appendix

Proposition 5.4.1. *Consider the solution $\Psi(x) = \operatorname{sech}(x)$ of the NLSE. The associated operator kernel $\boldsymbol{K}(x, y; \lambda)$ as defined in (4.211) is infinitely continuously-differentiable almost everywhere.*

Proof. Without loss of generality, we consider the case where $\lambda \neq 0$, and where $\operatorname{Re}(\nu) < \operatorname{Re}(\mu)$, where eigenvalues $\mu = \sqrt{1-2i\lambda}$ and $\nu = \sqrt{1+2i\lambda}$.

Our kernel is given by

$$\mathbf{K}(x,y) = \begin{cases} -\mathbf{R}_r(x)\mathbf{Q}e^{\mathbf{A}_\infty(x-y)}\mathbf{Q}\mathbf{R}_\ell(y), & x \geq y, \\ \mathbf{R}_r(x)(\mathbf{I}-\mathbf{Q})e^{\mathbf{A}_\infty(x-y)}(\mathbf{I}-\mathbf{Q})\mathbf{R}_\ell(y), & x < y. \end{cases} \tag{5.138}$$

Calling the first equation $\mathbf{K}_Q(x,y)$ and the second $\mathbf{K}_{IQ}(x,y)$, we can see that

$$\begin{aligned} \mathbf{K}_Q(x,y) &= -\mathbf{R}_r(x)\mathbf{P}\widehat{\mathbf{Q}}e^{\mathbf{D}(x-y)}\widehat{\mathbf{Q}}\mathbf{P}^{-1}\mathbf{R}_\ell(y), & (5.139) \\ \mathbf{K}_{IQ}(x,y) &= \mathbf{R}_r(x)\mathbf{P}(\mathbf{I}-\widehat{\mathbf{Q}})e^{\mathbf{D}(x-y)}(\mathbf{I}-\widehat{\mathbf{Q}})\mathbf{P}^{-1}\mathbf{R}_\ell(y), & (5.140) \end{aligned}$$

where we recall that $\mathbf{A}_\infty(\lambda) = \mathbf{PDP^{-1}}$, and $\mathbf{Q} = \mathbf{P}\widehat{\mathbf{Q}}\mathbf{P}^{-1}$ Let

$$\begin{aligned} \mathbf{R}_r(x) &= \begin{bmatrix} \mathbf{r}(x) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \ \mathbf{R}_\ell(x) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{L}(x) & \mathbf{0} \end{bmatrix}, \ \mathbf{P} = \begin{bmatrix} \mathbf{P}_1 & \mathbf{P}_2 \\ \mathbf{P}_3 & \mathbf{P}_4 \end{bmatrix}, \ \mathbf{P}^{-1} = \begin{bmatrix} \mathbf{S}_1 & \mathbf{S}_2 \\ \mathbf{S}_3 & \mathbf{S}_4 \end{bmatrix}, \\ \mathbf{D} &= \begin{bmatrix} \mathbf{D}_- & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_+ \end{bmatrix}, \ \widehat{\mathbf{Q}} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \text{ and } (\mathbf{I}-\widehat{\mathbf{Q}}) = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}. \end{aligned}$$

Then

$$\mathbf{K}_Q(x,y) = \begin{bmatrix} \widehat{\mathbf{K}}_Q(x,y) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} -\mathbf{r}(x)\mathbf{P}_1 e^{\mathbf{D}_-(x-y)}\mathbf{S}_2\mathbf{L}(y) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}, \tag{5.141}$$

and

$$\mathbf{K}_{IQ}(x,y) = \begin{bmatrix} \widehat{\mathbf{K}}_{IQ}(x,y) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{r}(x)\mathbf{P}_2 e^{\mathbf{D}_+(x-y)}\mathbf{S}_4\mathbf{L}(y) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}. \tag{5.142}$$

The matrix $\mathbf{D}$ of eigenvalues of $\mathbf{A}_\infty$ is given by

$$\mathbf{D} = \begin{bmatrix} \mathbf{D}_- & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_+ \end{bmatrix} = \begin{bmatrix} -\mu & 0 & 0 & 0 \\ 0 & -\nu & 0 & 0 \\ 0 & 0 & \nu & 0 \\ 0 & 0 & 0 & \mu \end{bmatrix}, \tag{5.143}$$

and by (5.8) ,

$$\mathbf{P} = \begin{bmatrix} \mathbf{P}_1 & \mathbf{P}_2 \\ \mathbf{P}_3 & \mathbf{P}_4 \end{bmatrix} = \begin{bmatrix} -\frac{i}{\mu} & \frac{i}{\nu} & -\frac{i}{\nu} & \frac{i}{\mu} \\ -\frac{1}{\mu} & -\frac{1}{\nu} & \frac{1}{\nu} & \frac{1}{\mu} \\ i & -i & -i & i \\ 1 & 1 & 1 & 1 \end{bmatrix}, \tag{5.144}$$

$$\mathbf{P}^{-1} = \begin{bmatrix} \mathbf{S}_1 & \mathbf{S}_2 \\ \mathbf{S}_3 & \mathbf{S}_4 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} i\mu & -\mu & -i & 1 \\ -i\nu & -\nu & i & 1 \\ i\nu & \nu & i & 1 \\ -i\mu & \mu & -i & 1 \end{bmatrix}. \tag{5.145}$$

In the case of the sech solution of the NLSE, $\mathbf{r}(x)$ and $\mathbf{L}(x)$ are diagonal, such that

$$\mathbf{r}(x) = \begin{bmatrix} \sqrt{3}\,\mathrm{sech}(x) & 0 \\ 0 & \mathrm{sech}(x) \end{bmatrix}, \ \mathbf{L}(x) = \begin{bmatrix} -2\sqrt{3}\,\mathrm{sech}(x) & 0 \\ 0 & -2\,\mathrm{sech}(x) \end{bmatrix}. \tag{5.146}$$

This gives that

$$\widehat{\mathbf{K}}_Q = \mathrm{sech}(x)\,\mathrm{sech}(y) \begin{bmatrix} -6\left(\frac{e^{-\mu(x-y)}}{\mu} + \frac{e^{-\nu(x-y)}}{\nu}\right) & -2\sqrt{3}i\left(\frac{e^{-\mu(x-y)}}{\mu} - \frac{e^{-\nu(x-y)}}{\nu}\right) \\ 2\sqrt{3}i\left(\frac{e^{-\mu(x-y)}}{\mu} - \frac{e^{-\nu(x-y)}}{\nu}\right) & -2\left(\frac{e^{-\mu(x-y)}}{\mu} + \frac{e^{-\nu(x-y)}}{\nu}\right) \end{bmatrix}, \tag{5.147}$$

and similarly that

$$\widehat{\mathbf{K}}_{IQ} = \mathrm{sech}(x)\,\mathrm{sech}(y) \begin{bmatrix} -6\left(\frac{e^{\mu(x-y)}}{\mu} + \frac{e^{\nu(x-y)}}{\nu}\right) & -2\sqrt{3}i\left(\frac{e^{\mu(x-y)}}{\mu} - \frac{e^{\nu(x-y)}}{\nu}\right) \\ 2\sqrt{3}i\left(\frac{e^{\mu(x-y)}}{\mu} - \frac{e^{\nu(x-y)}}{\nu}\right) & -2\left(\frac{e^{\mu(x-y)}}{\mu} + \frac{e^{\nu(x-y)}}{\nu}\right) \end{bmatrix}. \tag{5.148}$$

Clearly, $\mathbf{K}(x,y)$ is continuous across the diagonal $x = y$. Furthermore, for $\lambda \notin \sigma_{\mathrm{ess}}(\mathcal{L})$, μ, $\nu \neq 0$, and so $\mathbf{K}(x,y)$ is C^∞ almost everywhere (away from the diagonal). A similar result holds for the cases where $\mathrm{Re}(\nu) > \mathrm{Re}(\mu)$ or where $\lambda = 0$.

□

CHAPTER 6

CONCLUSION

In this dissertation, we first surveyed results from Fredholm [25] and Simon [24] about the regular Fredholm determinant and 2−modified Fredolm determinant of trace class and Hilbert-Schmidt operators evaluated on finite intervals which are expressed in terms of scalar-valued kernels. We extended these results to the case of trace class and Hilbert-Schmidt operators evaluated on the real line, which are expressed in terms of matrix-valued kernels. Following the work of Bornemann [26] in which he provided a formula for a numerical approximation of a trace class operator with scalar-valued kernel on a compact interval, we derived a formula for a numerical approximation of the 2−modified Fredholm determinant of a Hilbert-Schmidt operator with matrix-valued kernel on the real line. In order to approximate the regular and modified Fredholm determinant, we truncated the real line to a finite interval and then applied a composite Simpson's quadrature rule to approximate the integrals in the formula for the Fredholm determinant. Furthermore, we derived novel bounds on the errors related to these truncation and quadrature approximations.

While the Birman-Schwinger operators associated with solutions of the CQ-CGLE and NLSE have generally been treated as only being Hilbert-Schmidt, rather than satisfying the more stringent trace class condition, we were able to present criteria under which such operator kernels are trace class. Building off of results of Fredholm [25], Gohberg et. al [30], and Weidmann [31], we were able to show that under certain regularity conditions on the soliton solution Ψ, these Hilbert-Schmidt operators are, indeed, trace class. To do so, we extended the classical theory to the case of non-Hermitian Hilbert-Schmidt kernels on the real line given in terms of matrix-valued kernels.

We then applied our results on trace class and Hilbert-Schmidt operators and their respective Fredholm determinants to the specific case of the CQ-CGLE. Following the work of Gesztesy, Makarov, and Latushkin [20], and Zweck, Marzuola, and Jones [22], we presented the linearization of the CQ-CGLE about a soliton solution and derived the associated matrix-valued ODE system. Using an analytical formula for the essential spectrum of the linearized operator [22], we derived the Birman-Schwinger kernel, the roots of whose determinant correspond to the point spectrum of the linearized operator. We were able to apply our result that sufficiently regular Hilbert-Schmidt operators are trace class to the special case of the CQ-CGLE, and we showed that under suitable conditions, we could provide bounds on the numerical error in approximating the associated Fredholm determinants.

To test our results, we considered a known solution of the NLSE and derived an explicit formula for the matrix-valued kernel in this case. We showed that this solution satisfied all the necessary criteria for guaranteeing that the associated Birman-Schwinger operator is trace class. In addition, we derived an analytical formula for the Evans function associated with this solution. Using our trace class result, coupled with the fact that for trace class operator kernels of the CQ-CGLE and NLSE, the Fredholm determinant is equal to the Evans function, we were able to evaluate the error between our numerical approximation and the true Fredholm determinant.

We conducted numerical tests using the known solution of the NLSE and compared our theoretical results with those observed in practice. In our numerical simulations, we showed agreement between the truncation and quadrature error bounds we derived and those exhibited by our numerical scheme. In fact, for certain solutions, we show that a quadrature error can be achieved that is even better than the theoretical bound. We quantified the error between our numerically approximated determinants and the true determinants for known eigenvalues of the linearized system, and we observed the differences in behavior of the Fredholm and $2-$modified Fredholm determinants near the essential spectrum of the Birman-Schwinger operator. We also studied how the numerically computed Fredholm determinants depended on the quadrature method step size, the width of the truncation interval, and the accuracy of the composite Simpson's rule.

With the confidence gained in our method for numerically approximating the Fredholm and modified Fredholm determinant, we look forward to extending our research. A first direction for future work is to use this method in partner with a numerical optimization scheme to locate eigenvalues of linearized operators. After achieving this for known stationary solutions, we will be in the position to apply the same procedure to determine stability of stationary solutions found using a numerical split-step method. We hope to then perform parameter variation studies on these numerically-located solitons to optimize the parameters in the laser system. It is our ultimate goal to then apply this method for determining stability of pulses using Fredholm determinants to the case of periodically stationary solutions, a feat which is not likely achievable using an Evans function method.

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Papers (In Preparation):

- **E. Gallo**, J. Zweck, and Y. Latushkin. *"Numerical Fredholm Determinants for Matrix-Valued Kernels on the Real Line"*
- **E. Gallo**, J. Zweck, and Y. Latushkin. *"Stability of Ginzburg-Landau Pulses via Fredholm Determinants of Birman-Schwinger Operators"*
- J. Zweck, **E. Gallo**, and Y. Latushkin. *"A Regularity Condition Under Which Matrix and Operator Valued Kernels Define Trace Class Operators"*

Presentations:

- **E. Gallo**, J. Zweck, and Y. Latushkin. 2022. "Stability of Ginzburg-Landau Solitons via Fredholm Determinants of a Green's Operator." *5th Annual Meeting of the SIAM Texas-Louisiana Section, University of Houston,* Houston, TX, Nov. 4-6.
- **E. Gallo**, J. Zweck, and Y. Latushkin. 2022. "Stability of Ginzburg-Landau Solitons via Fredholm Determinants of a Green's Operator." *Computational Science Seminar, Department of Mathematical Sciences, The University of Texas at Dallas,* Richardson, TX, Oct. 28.