# DERIVATIVES OF (MODIFIED) FREDHOLM DETERMINANTS AND STABILITY OF STANDING AND TRAVELING WAVES

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Abstract. Continuing a line of investigation initiated in [11] exploring the connections between Jost and Evans functions and (modified) Fredholm determinants of Birman–Schwinger type integral operators, we here examine the stability index, or sign of the first nonvanishing derivative at frequency zero of the characteristic determinant, an object that has found considerable use in the study by Evans function techniques of stability of standing and traveling wave solutions of partial differential equations (PDE) in one dimension. This leads us to the derivation of general perturbation expansions for analytically-varying modified Fredholm determinants of abstract operators. Our main conclusion, similarly in the analysis of the determinant itself, is that the derivative of the characteristic Fredholm determinant may be efficiently computed from first principles for integral operators with semi-separable integral kernels, which include in particular the general one-dimensional case, and for sums thereof, which latter possibility appears to offer applications in the multi-dimensional case.

A second main result is to show that the multi-dimensional characteristic Fredholm determinant is the renormalized limit of a sequence of Evans functions defined in [23] on successive Galerkin subspaces, giving a natural extension of the one-dimensional results of [11] and answering a question of [27] whether this sequence might possibly converge (in general, no, but with renormalization, yes). Convergence is useful in practice for numerical error control and acceleration.

## 1. Introduction

A problem of general interest is to determine the spectrum of a general variable-coefficient linear differential operator $L = \sum_{|\alpha|=0}^{N} a_\alpha(x)\partial_x^\alpha$, $a_\alpha(x) \in \mathbb{R}^{n\times n}$, $x \in \mathbb{R}^d$, with prescribed behavior of the coefficients as $|x| \to \infty$. This arises naturally, for example, in the study of traveling- or standing-wave solutions of nonlinear PDEs in a wide variety of applications, as described, for example, in the survey articles [35], [47], and the references therein. In the one-dimensional case, $d = 1$, a very useful and general tool for this purpose is the *Evans function* [1], [6]–[9], [30], defined as a Wronskian $\mathcal{E}(z)$ of bases of the set of solutions $\Psi_\pm$ of the associated eigenvalue ODE $(L - \lambda)\Psi = 0$ decaying at $x = +\infty$ and $x = -\infty$, respectively, whose zeros correspond in location and multiplicity with the eigenvalues of $L$.

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Among the many applications of the Evans function, perhaps the simplest and most general is the computation of the *stability index*

$$\Gamma = \operatorname{sgn}\left(d_z^k \mathcal{E}(0)\right) \operatorname{sgn}(\mathcal{E}(+\infty)), \tag{1.1}$$

whose sign determines the parity of the number of unstable eigenvalues $\lambda$, or eigenvalues with positive real part $\operatorname{Re}(\lambda) > 0$, where $d_z^k \mathcal{E}(0)$ is the first nonvanishing derivative of $\mathcal{E}(z)$ at $z = 0$; see, for example, [9], [30], [47]. (A standard property of the Evans function is that it may be constructed so as to respect complex conjugation; in particular, it may be taken real-valued for $z \in \mathbb{R}$.) A problem that has received considerable recent interest[1] is to extend the Evans function, and in particular the stability index, to the more general setting of multi-dimensions in a way that is useful for practical computations. Here, we refer mainly to numerical computation, as presumably the only feasible way to treat large-scale problems associated with multi-dimensions.

Various different constructions have been suggested toward this end; see, for example, [3], [4], [23]. However, only one of these, the Galerkin approximation method of [23] (described in Section 4), seems in principle computable, and the computations involved appear quite numerically intensive. (So far, no such computations have satisfactorily been carried out, though, see the proposed methods discussed in [18], [27].) It is therefore highly desirable to explore other directions that may be more computationally efficient.

Here, we follow a very natural direction first proposed in [11]. Specifically, it is shown in [11] for a quite general class of one-dimensional operators $L$ that the Evans function, appropriately normalized, agrees with a (modified) characteristic *Fredholm determinant*, thus generalizing the classical relation known for the *Jost function* associated with Schrödinger operators of mathematical physics; for further discussion of this problem and its history, see [11] and references therein. A central point of the analysis is the observation [13] that *semi-separability* of the integral kernel of the resolvent operator is the key property of one-dimensional operators that makes possible the reduction of the infinite-dimensional characteristic determinant to a finite-dimensional determinant expressed by the Jost or Evans function.

The identification of Evans functions and Fredholm determinants yields a natural generalization of the Evans function to multi-dimensions, since the definition of (modified) Fredholm determinants extends to higher-dimensional problems. What is not immediately clear is whether this extension leads to a practically useful, computable formulation of either the Evans function or the stability index. For, up to now, the main approach to computation of the characteristic determinant was to express it as a Jost function or the usual, Wronskian expression for the (one-dimensional) Evans function.

In the present paper, we extend some of the investigations of [11] in two ways. First, we derive in Theorem 2.7 a general perturbation formula for analytically-varying modified Fredholm determinants, by which we may express the stability index as a product of a finite-dimensional minor (Lyapunov–Schmidt decomposition) and a finite-rank perturbation of the original characteristic determinant: that is, directly in terms of Fredholm determinants, without reference to a Jost or Evans

[1]For example, this was a focus topic of the workshop "Stability Criteria for Multi-Dimensional Waves and Patterns", at the American Institute of Mathematics (AIM) in Palo Alto (California/USA), May 16-20, 2005.

function formulation. This is carried out in Section 2, with the main result given in Theorems 2.3 and 2.7.

Second, we discuss in Theorem 3.8 an important case when the finite-rank perturbation part, like the original characteristic determinant, may be reduced to a finite-dimensional determinant whenever the resolvent of the operator $L$ has a semi-separable integral kernel, in particular, in the one-dimensional case. This is a consequence of the simple observation that a sum of operators with semi-separable integral kernels may be expressed as an operator with a matrix-valued semi-separable integral kernel and evaluated in the same way; indeed, the analysis of [13] on which this reduction is based is actually presented in the more general, matrix-valued setting. We illustrate this procedure in Section 3 by explicit computations for the example of a scalar Schrödinger operator that arises in the study of stability of standing-wave patterns of one-dimensional reaction–diffusion equations, in the process illuminating various relations between Jost functions and characteristic Fredholm determinants.

To explain our main results in Section 3, we recall that a classical formula by Jost and Pais equates the Jost function and the Fredholm determinant of a Birman–Schwinger-type operator (cf. Section 3 for its discussion and definitions). Since the Jost function is the Wronskian of the Jost solutions $\Psi_\pm$, this result can be viewed as a calculation of the Fredholm determinant via the solutions $\Psi_\pm$ of the homogenous Schrödinger equation that are asymptotic to the exponential plane waves. We proved a new formula in this spirit, see (3.99), and computed the *derivative* of the Jost function, that is, the derivative of the Fredholm determinant, via some solutions $\psi_\pm$ of a *nonhomogenous* Schrödinger equation (cf. (3.127)) that, in turn, are asymptotic to $\Psi_\pm$ (cf. (3.100)). We are not aware of any earlier references mentioning these solutions $\psi_\pm$.

In addition, we obtain in Section 3 in passing an elementary proof of an interesting formula derived by Simon [37] for the Jost solutions $\Psi_\pm(z,\,\cdot\,)$ in terms of Fredholm determinants.

Of course, the approach of Section 3 applies equally well to the general one-dimensional case, yielding in principle a similarly compact formula for the stability index obtained entirely through Fredholm determinant manipulations. However, in this paper we do not pursue this any further, leaving this topic for future research.

More generally, this suggests an approach to the multi-dimensional case by a limiting procedure based on Galerkin approximation, but carried out within the Fredholm determinant framework. More precisely, we propose in place of the standard approach of reducing to a large one-dimensional system by Galerkin approximation then defining a standard Evans function, to first relate the Evans function and a Fredholm determinant, then evaluate the latter by Galerkin approximation/semi-separable reduction. This offers the advantage that successive levels of approximation are embedded in a hierarchy of convergent problems useful for error control, without the need to prescribe appropriate normalizations by hand.

Our main result in the multi-dimensional case, generalizing the one-dimensional results of [11], is that the sequence of approximate 2-modified Jost functions $\mathcal{F}_{2,J}$ generated by Galerkin approximation of the 2-modified Fredholm determinant at wave number $J$ *agrees, up to appropriate normalization*, with the Evans functions $\mathcal{E}_J$ constructed in [23] for the sequence of one-dimensional equations obtained by Galerkin approximation at the same wave number; see Theorem 4.15. This includes the information that the sequence $\mathcal{E}_J$, introduced in [23] as a tool to compute a topologically-defined stability index, in fact determines a well-defined 2-modified Jost function; that is, an appropriate renormalization $\mathcal{F}_{2,J} = e^{\Theta_J}\mathcal{E}_J$ of the sequence $\mathcal{E}_J$ converges to a limiting 2-modified Jost function $\mathcal{F}_2$ (cf. Theorem 4.9), a fact that is not apparent from the construction of [23]. The Jost and Evans functions of course carry considerably more information than the stability index alone.

We obtain at the same time a slightly different algorithm for computing the stability index, which avoids some logistical difficulties of the existing Galerkin schemes. We discuss these issues in Section 4, illustrating with respect to the basic multi-dimensional examples of flow in an infinite cylinder and solutions with radial limits.

Finally, we note that the ODE systems arising in computation of the Galerkin-based Evans functions $\mathcal{E}_J$ become extremely stiff as $J \to \infty$, featuring growth/decay modes of order $\pm J$. Thus, numerical conditioning becomes a crucial consideration for the large-scale systems that result in multi-dimensions ($J \sim 100$, as described in [18]). It may well be that, for sufficiently large $J$, direct computation of the Fredholm determinant by discretization may be more efficient than either Evans function computations or simple discretization of the linearized operator $L$; see Subsection 4.1.7. Efficient numerical realization of this approach would be a very interesting direction for future investigation.

**Plan of the paper.** In Section 2, we provide a general perturbation formula for analytically varying (modified) Fredholm determinants. In Section 3, we use this result together with the reduction method of [13] to compute the stability index in the case of a one-dimensional real Schrödinger operator. Finally, in Section 4, we describe extensions to multi-dimensions.

## 2. A general perturbation expansion for Fredholm Determinants

In this section we describe the analytic behavior of Fredholm determinants $\det_{\mathcal{H}}(I - A(z))$ and modified Fredholm determinants $\det_{2,\mathcal{H}}(I - A(z))$ in a neighborhood of $z = 0$ with $A(\,\cdot\,)$ analytic in a neighborhood of $z = 0$ in trace norm, respectively, Hilbert–Schmidt norm. Special emphasis will be put on the case where $[I - A(0)]$ is not boundedly invertible in the Hilbert space $\mathcal{H}$.

In the first part of this section we suppose that all relevant operators belong to the trace class and consider the associated Fredholm determinants. In the second part we consider 2-modified Fredholm determinants in the case where the relevant operators are Hilbert–Schmidt operators.

### 2.1. Trace class operators.

In the course of the proof of our first result we repeatedly will have to use some of the standard properties of determinants, such as,

$$\det_{\mathcal{H}}((I_{\mathcal{H}} - A)(I_{\mathcal{H}} - B)) = \det_{\mathcal{H}}(I_{\mathcal{H}} - A)\det_{\mathcal{H}}(I_{\mathcal{H}} - B), \quad A, B \in \mathcal{B}_1(\mathcal{H}), \tag{2.1}$$

$$\det_{\mathcal{H}'}(I_{\mathcal{H}'} - AB) = \det_{\mathcal{H}}(I_{\mathcal{H}} - BA) \text{ for all } A \in \mathcal{B}(\mathcal{H}, \mathcal{H}'),\ B \in \mathcal{B}(\mathcal{H}', \mathcal{H}) \text{ such that } BA \in \mathcal{B}_1(\mathcal{H}),\ AB \in \mathcal{B}_1(\mathcal{H}'), \tag{2.2}$$

and

$$\det_{\mathcal{H}}(I_{\mathcal{H}} - A) = \det_{\mathbb{C}^k}(I_k - D_k) \text{ for } A = \begin{pmatrix} 0 & C \\ 0 & D_k \end{pmatrix},\ \mathcal{H} = \mathcal{K} \dotplus \mathbb{C}^k, \tag{2.3}$$

since

$$I_{\mathcal{H}} - A = \begin{pmatrix} I_{\mathcal{K}} & -C \\ 0 & I_k - D_k \end{pmatrix} = \begin{pmatrix} I_{\mathcal{K}} & 0 \\ 0 & I_k - D_k \end{pmatrix} \begin{pmatrix} I_{\mathcal{K}} & -C \\ 0 & I_k \end{pmatrix}. \tag{2.4}$$

Finally, assuming $A, B \in \mathcal{B}_1(\mathcal{H})$, we also mention the following estimates:

$$|\det_{\mathcal{H}}(I_{\mathcal{H}} - A)| \leq \exp(\|A\|_{\mathcal{B}_1(\mathcal{H})}), \tag{2.5}$$

$$|\det_{\mathcal{H}}(I_{\mathcal{H}} - A) - \det_{\mathcal{H}}(I_{\mathcal{H}} - B)| \leq \|A - B\|_{\mathcal{B}_1(\mathcal{H})} \times \exp(\|A\|_{\mathcal{B}_1(\mathcal{H})} + \|B\|_{\mathcal{B}_1(\mathcal{H})} + 1). \tag{2.6}$$

Here $\mathcal{H}$ and $\mathcal{H}'$ are complex separable Hilbert spaces, $\mathcal{B}(\mathcal{H})$ denotes the set of bounded linear operators on $\mathcal{H}$, $\mathcal{B}_p(\mathcal{H})$, $p \geq 1$, denote the usual trace ideals of $\mathcal{B}(\mathcal{H})$, and $I_{\mathcal{H}}$ denotes the identity operator in $\mathcal{H}$ (similarly, $I_k$ abbreviates the identity operator in $\mathbb{C}^k$). The ideal of compact operators on $\mathcal{H}$ will be denoted by $\mathcal{B}_\infty(\mathcal{H})$. Moreover, $\det_{p,\mathcal{H}}(I_{\mathcal{H}} - A)$, $A \in \mathcal{B}_p(\mathcal{H})$, denotes the ($p$-modified) Fredholm determinant of $I_{\mathcal{H}} - A$ with $\det_{1,\mathcal{H}}(I_{\mathcal{H}} - A) = \det_{\mathcal{H}}(I_{\mathcal{H}} - A)$, $A \in \mathcal{B}_1(\mathcal{H})$, the standard Fredholm determinant of a trace class operator, and $\operatorname{tr}_{\mathcal{H}}(A)$, $A \in \mathcal{B}_1(\mathcal{H})$, the trace of a trace class operator in $\mathcal{H}$. Finally, $\dotplus$ in (2.3) denotes a direct but not necessary orthogonal direct decomposition of $\mathcal{H}$ into $\mathcal{K}$ and the $k$-dimensional subspace $\mathbb{C}^k$. These results can be found, for instance, in [14], [17, Sect. IV.1], [32, Ch. 17], [36], [38, Ch. 3]. In the following, $\sigma(T)$ denotes the spectrum of a densely defined, closed linear operator $T$ in $\mathcal{H}$, and $\sigma_{\mathrm{d}}(T)$ denotes the discrete spectrum of $T$ (i.e., isolated eigenvalues of $T$ of finite algebraic multiplicity).

For the general theory of (modified) Fredholm determinants we refer, for instance, to [5, Sect. XI.9], [14], [15], [16, Ch. X.III], [17, Ch. IV], [36], and [38, Sects. 3, 9].

**Hypothesis 2.1.** *Suppose $A(\,\cdot\,) \in \mathcal{B}_1(\mathcal{H})$ is a family of trace class operators on $\mathcal{H}$ analytic on an open neighborhood $\Omega_0 \subset \mathbb{C}$ of $z = 0$ in trace class norm $\|\cdot\|_{\mathcal{B}_1(\mathcal{H})}$.*

Given Hypothesis 2.1 we write

$$A(z) \underset{z \to 0}{=} A_0 + A_1 z + O\big(z^2\big) \text{ for } z \in \Omega_0 \text{ sufficiently small, } A_\ell \in \mathcal{B}_1(\mathcal{H}),\ \ell = 0, 1. \tag{2.7}$$

We start by noting the following well-known result.

**Lemma 2.2.** *Assume Hypothesis 2.1 and suppose $(I_{\mathcal{H}} - A_0)^{-1} \in \mathcal{B}(\mathcal{H})$. Then,*

$$\det_{\mathcal{H}}(I_{\mathcal{H}} - A(z)) \underset{z \to 0}{=} \det_{\mathcal{H}}(I_{\mathcal{H}} - A_0) - \det_{\mathcal{H}}(I_{\mathcal{H}} - A_0)\operatorname{tr}_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)^{-1} A_1\big) z + O\big(z^2\big). \tag{2.8}$$

*Proof.* This follows from

$$\begin{aligned} \det_{\mathcal{H}}(I_{\mathcal{H}} - A(z)) &\underset{z \to 0}{=} \det_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)\big[I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1} A_1 z + O\big(z^2\big)\big]\big) \\ &\underset{z \to 0}{=} \det_{\mathcal{H}}(I_{\mathcal{H}} - A_0)\big[1 - \operatorname{tr}_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)^{-1} A_1\big) z + O\big(z^2\big)\big], \end{aligned} \tag{2.9}$$

where we used the fact that

$$\det_{\mathcal{H}}(I_{\mathcal{H}} - Bz) = \exp\bigg[-\sum_{k \in \mathbb{N}} \frac{\operatorname{tr}_{\mathcal{H}}\big(B^k\big)}{k} z^k\bigg] \text{ for } |z| \text{ sufficiently small} \tag{2.10}$$

with $B \in \mathcal{B}_1(\mathcal{H})$. $\square$

Next we turn to the case where $(I_{\mathcal{H}} - A_0)$ is not boundedly invertible. Before we state the analog of Lemma 2.2 in this more general setting, we need some preparations.

We temporarily assume

$$A_0 \in \mathcal{B}(\mathcal{H}) \text{ and } 1 \in \sigma_{\rm d}(A_0), \tag{2.11}$$

and abbreviate by $P_0$ the Riesz projection associated with $A_0$ and the discrete eigenvalue 1 of $A_0$,

$$P_0 = \frac{-1}{2\pi i} \oint_{\mathcal{C}_0} d\zeta \, (A_0 - \zeta I_{\mathcal{H}})^{-1}, \tag{2.12}$$

where $\mathcal{C}_0$ denotes a sufficiently small counterclockwise oriented circle centered at 1 such that no part of $\sigma(A_0)\backslash\{1\}$ intersects $\mathcal{C}_0$ and its open interior. We denote by

$$n_0 = \dim(\operatorname{ran}(P_0)) \tag{2.13}$$

the algebraic multiplicity of the eigenvalue 1 of $A_0$. In addition, we introduce the quasinilpotent operator $D_0$ associated with $A_0$ and its discrete eigenvalue 1 by

$$D_0 = (A_0 - I_{\mathcal{H}})P_0 \tag{2.14}$$

such that

$$D_0 = D_0 P_0 = P_0 D_0 = P_0 D_0 P_0. \tag{2.15}$$

In the following we denote by $\Delta(z_0; r_0) \subset \mathbb{C}$ the open disc centered at $z_0 \in \mathbb{C}$ of radius $r_0 > 0$ and by $\mathcal{C}(z_0; r_0) = \partial\Delta(z_0; r_0)$ the counterclockwise oriented circle of radius $r_0 > 0$ centered at $z_0$. Assuming that the analytic family of operators $A(\cdot)$ satisfies Hypothesis 2.1, we prescribe an $\varepsilon_0 > 0$ and choose a sufficiently small open neighborhood $\Omega_0$ of $z = 0$ such that all eigenvalues $\lambda_j(z)$ of $A(z)$ for $z \in \Omega_0$, which satisfy $\lambda_j(0) = 1$, $1 \leq j \leq \nu_0$ for some $\nu_0 \in \mathbb{N}$ with $\nu_0 \leq n_0$, stay in the disc $\Delta(1; \varepsilon_0/2)$. Moreover we assume that $\Omega_0$ is chosen sufficiently small that no other eigenvalue branches of $A(z)$, $z \in \Omega_0$, intersect the larger disc $\Delta(1; \varepsilon_0)$. Introducing the Riesz projection $P(z)$ associated with $A(z)$, $z \in \Omega_0$ (cf., e.g, [21, Sect. III.6]),

$$P(z) = \frac{-1}{2\pi i} \oint_{\mathcal{C}(1;\varepsilon_0)} d\zeta \, (A(z) - \zeta I_{\mathcal{H}})^{-1}, \quad z \in \Omega_0, \tag{2.16}$$

then $P(\cdot)$ is analytic in $\Omega_0$ and we expand

$$P(z) \underset{z \to 0}{=} P_0 + P_1 z + O\big(z^2\big) \text{ for } |z| \text{ sufficiently small.} \tag{2.17}$$

Moreover, we introduce the projections

$$Q(z) = I_{\mathcal{H}} - P(z), \quad z \in \Omega_0, \quad Q_0 = I_{\mathcal{H}} - P_0, \tag{2.18}$$

and expand

$$Q(z) \underset{z \to 0}{=} Q_0 + Q_1 z + O\big(z^2\big) \text{ for } |z| \text{ sufficiently small.} \tag{2.19}$$

Since $P(z)^2 = P(z)$, (2.17) implies

$$P_0 P_1 + P_1 P_0 = P_1 \text{ and hence } P_0 P_1 P_0 = 0. \tag{2.20}$$

Following Wolf [45] we now introduce the transformation

$$T(z) = P_0 P(z) + Q_0 Q(z) = P_0 P(z) + [I_{\mathcal{H}} - P_0][I_{\mathcal{H}} - P(z)], \quad z \in \Omega_0, \tag{2.21}$$

such that

$$P_0 T(z) = T(z) P(z), \quad Q_0 T(z) = T(z) Q(z), \quad z \in \Omega_0. \tag{2.22}$$

In addition, for $|z|$ sufficiently small,

$$T(z) \underset{z\to 0}{=} I_{\mathcal{H}} + (P_0P_1 - P_1P_0)z + O\big(z^2\big), \tag{2.23}$$

$$T(z)^{-1} \underset{z\to 0}{=} I_{\mathcal{H}} - (P_0P_1 - P_1P_0)z + O\big(z^2\big), \tag{2.24}$$

and hence

$$P_0 = T(z)P(z)T(z)^{-1}, \quad Q_0 = T(z)Q(z)T(z)^{-1} \tag{2.25}$$

for $|z|$ sufficiently small. Below we will use (2.25) to reduce determinants in the Hilbert space $P(z)\mathcal{H}$ to that in the fixed Hilbert space $P_0\mathcal{H}$.

Next, we introduce the following notation: We denote by $S \in \mathcal{B}\big(P_0\mathcal{H}, \mathbb{C}^{n_0}\big)$ the boundedly invertible linear operator which puts the nilpotent operator $P_0D_0P_0$ into its $n_0 \times n_0$ Jordan canonical form $SP_0D_0P_0S^{-1}$, and abbreviate by $\nu_0$ the number of entries 1 in the canonical Jordan representation of $SP_0D_0P_0S^{-1}$, where[2] $0 \leq \nu_0 \leq n_0 - 1$. Moreover, we denote by $\widetilde{A}_1$ the $(n_0 - \nu_0) \times (n_0 - \nu_0)$-matrix obtained from $SP_0A_1P_0S^{-1}$ by striking from it the $\nu_0$ columns and rows in which $SP_0D_0P_0S^{-1}$ contains an entry 1. With this notation in mind, we now formulate our first abstract result on expansions of Fredholm determinants $\det_{\mathcal{H}}(I_{\mathcal{H}} - A(z))$ as $z \to 0$, with $[I_{\mathcal{H}} - A(0)]$ not boundedly invertible in $\mathcal{H}$:

**Theorem 2.3.** *Assume Hypothesis* 2.1 *and let* $1 \in \sigma_{\rm d}(A_0)$. *Then, given the notation in the paragraph preceding this theorem,*

$$\begin{aligned}
\det{}_{\mathcal{H}}(I_{\mathcal{H}} - A(z)) &\underset{z\to 0}{=} \big[\det{}_{Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) + O(z)\big] \\
&\qquad \times (-1)^{n_0} \det{}_{P_0\mathcal{H}}(P_0D_0P_0 + P_0[A_1 + O(z)]P_0 z) \\
&\underset{z\to 0}{=} \det{}_{Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) \det{}_{\mathbb{C}^{n_0-\nu_0}}\big(\widetilde{A}_1\big)(-z)^{n_0-\nu_0} + O\big(z^{n_0-\nu_0+1}\big).
\end{aligned} \tag{2.26}$$

*In the special case where* 1 *is a semisimple eigenvalue of* $A_0$ *(i.e., where* $D_0 = 0$ *and* $\nu_0 = 0$*) one obtains,*

$$\begin{aligned}
\det{}_{\mathcal{H}}(I_{\mathcal{H}} - A(z)) &\underset{z\to 0}{=} \det{}_{Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) \det{}_{P_0\mathcal{H}}(P_0A_1P_0)(-z)^{n_0} + O\big(z^{n_0+1}\big) \\
&\underset{z\to 0}{=} \det{}_{\mathcal{H}}(I_{\mathcal{H}} - P_0 - A_0) \det{}_{P_0\mathcal{H}}(P_0A_1P_0) z^{n_0} + O\big(z^{n_0+1}\big).
\end{aligned} \tag{2.27}$$

*In particular, if* 1 *is a simple eigenvalue of* $A_0$ *(i.e., if* $n_0 = 1$, $D_0 = 0$, *and* $\nu_0 = 0$*), one obtains*

$$\det{}_{\mathcal{H}}(I_{\mathcal{H}} - A(z)) \underset{z\to 0}{=} \det{}_{\mathcal{H}}(I_{\mathcal{H}} - P_0 - A_0) \det{}_{P_0\mathcal{H}}(P_0A_1P_0) z + O\big(z^2\big). \tag{2.28}$$

*Proof.* Since

$$\mathcal{H} = P(z)\mathcal{H} \dotplus Q(z)\mathcal{H}, \quad P(z)A(z) = A(z)P(z), \quad P(z)Q(z) = Q(z)P(z) = 0, \tag{2.29}$$

one computes using (2.22),

$$\begin{aligned}
\det{}_{\mathcal{H}}(I_{\mathcal{H}} - A(z)) &= \det{}_{\mathcal{H}}\big(I_{\mathcal{H}} - T(z)A(z)T(z)^{-1}\big) \\
&= \det{}_{\mathcal{H}}\big(I_{\mathcal{H}} - T(z)[P(z)A(z)P(z) + Q(z)A(z)Q(z)]T(z)^{-1}\big) \\
&= \det{}_{\mathcal{H}}\big(I_{\mathcal{H}} - P_0T(z)A(z)T(z)^{-1}P_0 - Q_0T(z)A(z)T(z)^{-1}Q_0\big)
\end{aligned}$$

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[2]In particular, $\nu_0$ equals the sum of the dimensions of all nontrivial (i.e., nondiagonal) Jordan blocks in the canonical Jordan representation $SP_0D_0P_0S^{-1}$ of $P_0D_0P_0$. Thus, $SP_0D_0P_0S^{-1}$ contains $\nu_0$ entries 1 at certain places right above the main diagonal and 0's everywhere else including on the main diagonal.

$$\begin{aligned}&= \det_{P_0\mathcal{H}}\big(I_{P_0\mathcal{H}} - P_0T(z)A(z)T(z)^{-1}P_0\big)\\ &\quad \times \det_{Q_0\mathcal{H}}\big(I_{Q_0\mathcal{H}} - Q_0T(z)A(z)T(z)^{-1}Q_0\big). \end{aligned} \tag{2.30}$$

Using (2.20), (2.7), (2.23), and (2.24), one computes

$$P_0T(z)A(z)T(z)^{-1}P_0 \underset{z\to 0}{=} P_0A_0P_0 + P_0A_1P_0z + P_0O\big(z^2\big)P_0, \tag{2.31}$$

$$Q_0T(z)A(z)T(z)^{-1}Q_0 \underset{z\to 0}{=} Q_0A_0Q_0 + Q_0O(z)Q_0 \tag{2.32}$$

for $|z|$ sufficiently small. Relation (2.32) implies

$$\det_{Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0T(z)A(z)T(z)^{-1}Q_0) \underset{z\to 0}{=} \det_{Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) + O(z) \neq 0 \tag{2.33}$$

for $|z|$ sufficiently small, and hence we next focus on the first factor on the right-hand side of (2.30). Applying (2.14), (2.15), and (2.31) one obtains

$$\begin{aligned}&\det_{P_0\mathcal{H}}\big(I_{P_0\mathcal{H}} - P_0T(z)A(z)T(z)^{-1}P_0\big)\\ &\quad\underset{z\to 0}{=} \det_{P_0\mathcal{H}}(I_{P_0\mathcal{H}} - P_0A_0P_0 - P_0[A_1 + O(z)]P_0z)\\ &\quad\underset{z\to 0}{=} (-1)^{n_0}\det_{P_0\mathcal{H}}(P_0D_0P_0 + P_0[A_1 + O(z)]P_0z). \end{aligned} \tag{2.34}$$

Next, let $S \in \mathcal{B}\big(P_0\mathcal{H}, \mathbb{C}^{n_0}\big)$ be the transformation which puts $P_0D_0P_0$ into its Jordan canonical form $\widehat{D}_0 = SP_0D_0P_0S^{-1}$ and denote

$$\widehat{A}_1(z) \underset{z\to 0}{=} SP_0[A_1 + O(z)]P_0S^{-1} \underset{z\to 0}{=} \widehat{A}_1 + O(z). \tag{2.35}$$

Then,

$$\begin{aligned}&\det_{P_0\mathcal{H}}\big(I_{P_0\mathcal{H}} - P_0T(z)A(z)T(z)^{-1}P_0\big)\\ &\quad\underset{z\to 0}{=} (-1)^{n_0}\det_{P_0\mathcal{H}}(P_0D_0P_0 + P_0[A_1 + O(z)]P_0z)\\ &\quad\underset{z\to 0}{=} (-1)^{n_0}\det_{\mathbb{C}^{n_0}}\big(\widehat{D}_0 + \widehat{A}_1(z)z\big)\\ &\quad\underset{z\to 0}{=} (-1)^{n_0}\det_{\mathbb{C}^{n_0}}\big(\widehat{D}_0 + \widehat{A}_1z + O\big(z^2\big)\big)\\ &\quad\underset{z\to 0}{=} (-z)^{n_0-\nu_0}\det_{\mathbb{C}^{n_0-\nu_0}}\big(\widetilde{A}_1 + O(z)\big)\\ &\quad\underset{z\to 0}{=} (-z)^{n_0-\nu_0}\det_{\mathbb{C}^{n_0-\nu_0}}\big(\widetilde{A}_1\big) + O\big(z^{n_0-\nu_0+1}\big), \end{aligned} \tag{2.36}$$

by applying the Laplace determinant expansion formula (cf., e.g., [43, Sect. 3.3]) to $\det_{\mathbb{C}^{n_0}}\big(\widehat{D}_0 + \widehat{A}_1z + O\big(z^2\big)\big)$ with respect to the $\nu_0$ columns in $\widehat{D}_0$ which contain a 1. Combining (2.36) and (2.33) then proves (2.26).

If 1 is a semisimple eigenvalue of $A_0$ and hence $D_0 = 0$, $\nu_0 = 0$, the first line on the right-hand side in (2.27) is clear from (2.26). To prove the second line in the right-hand side of (2.27), we recall that

$$P_0A_0P_0 = P_0A_0 = A_0P_0 = P_0 \text{ and } Q_0A_0Q_0 = Q_0A_0 = (I_{\mathcal{H}} - P_0)A_0 = A_0 - P_0, \tag{2.37}$$

and hence,

$$\begin{aligned}\det_{\mathcal{H}}(I_{\mathcal{H}} - P_0 - A_0) &= \det_{\mathcal{H}}(I_{\mathcal{H}} - P_0 - P_0A_0P_0 - Q_0A_0Q_0)\\ &= \det_{\mathcal{H}}(-P_0 + Q_0 - Q_0A_0Q_0)\\ &= (-1)^{n_0}\det_{Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) \neq 0. \end{aligned} \tag{2.38}$$

The special case $n_0 = 1$ in (2.27) then yields (2.28). □

**Remark 2.4.** Since $\nu_0$ can take on any particular value from 0 to $n_0 - 1$ and $A_1$ is generally independent of $A_0$ and hence $D_0$, the power $n_0 - \nu_0$ of $z$ in (2.26) can take on any value between 1 and $n_0$.

2.2. **Hilbert–Schmidt operators.** Next, we treat the case of 2-modified Fredholm determinants, where all relevant operators are only assumed to lie in the Hilbert–Schmidt class. In addition to (2.1)–(2.3) we recall the following standard facts for 2-modified Fredholm determinants $\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A)$, $A \in \mathcal{B}_2(\mathcal{H})$ (cf., e.g., [15], [16, Ch. XIII], [17, Sect. IV.2], [36], [38, Ch. 3]),

$$\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A) = \det_{\mathcal{H}}((I_{\mathcal{H}} - A)\exp(A)), \quad A \in \mathcal{B}_2(\mathcal{H}), \tag{2.39}$$

$$\det_{2,\mathcal{H}}((I_{\mathcal{H}} - A)(I_{\mathcal{H}} - B)) = \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A)\det_{2,\mathcal{H}}(I_{\mathcal{H}} - B)\, e^{-\operatorname{tr}_{\mathcal{H}}(AB)}, \quad A, B \in \mathcal{B}_2(\mathcal{H}), \tag{2.40}$$

$$\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A) = \det_{\mathcal{H}}(I_{\mathcal{H}} - A)\, e^{\operatorname{tr}_{\mathcal{H}}(A)}, \quad A \in \mathcal{B}_1(\mathcal{H}), \tag{2.41}$$

$$\det_{2,\mathcal{H}'}(I_{\mathcal{H}'} - AB) = \det_{2,\mathcal{H}}(I_{\mathcal{H}} - BA) \text{ for all } A \in \mathcal{B}(\mathcal{H},\mathcal{H}'),\ B \in \mathcal{B}(\mathcal{H}',\mathcal{H}) \text{ such that } BA \in \mathcal{B}_2(\mathcal{H}),\ AB \in \mathcal{B}_2(\mathcal{H}'). \tag{2.42}$$

Moreover, in analogy to (2.10) one now has

$$\det_{2,\mathcal{H}}(I_{\mathcal{H}} - Bz) = \exp\bigg[-\sum_{k=2}^{\infty}\frac{\operatorname{tr}_{\mathcal{H}}\big(B^k\big)}{k}z^k\bigg] \text{ for } |z| \text{ sufficiently small, } B \in \mathcal{B}_2(\mathcal{H}). \tag{2.43}$$

Finally, assuming $A, B \in \mathcal{B}_2(\mathcal{H})$, we mention some estimates to be useful in Section 4: For some $C > 0$,

$$|\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A)| \le \exp\big(C\|A\|^2_{\mathcal{B}_2(\mathcal{H})}\big), \tag{2.44}$$

$$|\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A) - \det_{2,\mathcal{H}}(I_{\mathcal{H}} - B)| \le \|A - B\|_{\mathcal{B}_2(\mathcal{H})} \times \exp\big(C[\|A\|_{\mathcal{B}_2(\mathcal{H})} + \|B\|_{\mathcal{B}_2(\mathcal{H})} + 1]^2\big) \tag{2.45}$$

**Hypothesis 2.5.** *Suppose $A(\,\cdot\,) \in \mathcal{B}_2(\mathcal{H})$ is a family of Hilbert–Schmidt operators on $\mathcal{H}$ analytic on an open neighborhood $\Omega_0 \subset \mathbb{C}$ of $z = 0$ in the Hilbert–Schmidt norm $\|\cdot\|_{\mathcal{B}_2(\mathcal{H})}$.*

Given Hypothesis 2.5, we write again

$$A(z) \underset{z\to 0}{=} A_0 + A_1 z + O\big(z^2\big) \text{ for } z \in \Omega_0 \text{ sufficiently small, } A_\ell \in \mathcal{B}_2(\mathcal{H}),\ \ell = 0, 1. \tag{2.46}$$

We start with the analog of Lemma 2.2.

**Lemma 2.6.** *Assume Hypothesis 2.5 and suppose $(I_{\mathcal{H}} - A_0)^{-1} \in \mathcal{B}(\mathcal{H})$. Then,*

$$\begin{aligned}\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A(z)) \underset{z\to 0}{=} &\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0) \\ &- \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)\operatorname{tr}_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)^{-1}A_0A_1\big)z + O\big(z^2\big).\end{aligned} \tag{2.47}$$

*Proof.* This follows most easily from rewriting (2.8) in terms of modified Fredholm determinants $\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \cdot\,)$, using (2.41), and then approximating Hilbert–Schmidt operators by trace class (or finite-rank) operators (cf., e.g., [17, Theorem III.7.1]). Indeed, one computes using (2.41) repeatedly,

$$\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A(z)) = \det_{\mathcal{H}}(I_{\mathcal{H}} - A(z))e^{\operatorname{tr}_{\mathcal{H}}(A(z))}$$

$$
\begin{aligned}
&= \det_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)\big[I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}(A(z) - A_0)\big]\big)e^{\operatorname{tr}_{\mathcal{H}}(A(z))} \\
&= \det_{\mathcal{H}}(I_{\mathcal{H}} - A_0)\det_{\mathcal{H}}\big(I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}(A(z) - A_0)\big)e^{\operatorname{tr}_{\mathcal{H}}(A(z))} \\
&= \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)e^{-\operatorname{tr}_{\mathcal{H}}(A_0)}\det_{2,\mathcal{H}}\big(I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}(A(z) - A_0)\big) \\
&\quad \times e^{-\operatorname{tr}_{\mathcal{H}}((I_{\mathcal{H}} - A_0)^{-1}(A(z)-A_0))}e^{\operatorname{tr}_{\mathcal{H}}(A(z))} \\
&= \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)\det_{2,\mathcal{H}}\big(I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}(A(z) - A_0)\big) \\
&\quad \times e^{\operatorname{tr}_{\mathcal{H}}([I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}](A(z)-A_0))} \\
&= \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)\det_{2,\mathcal{H}}\big(I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}(A(z) - A_0)\big) \\
&\quad \times e^{-\operatorname{tr}_{\mathcal{H}}((I_{\mathcal{H}} - A_0)^{-1}A_0(A(z)-A_0))} \\
&\underset{z\to 0}{=} \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)\det_{2,\mathcal{H}}\big(I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}A_1 z + O\big(z^2\big)\big) \\
&\quad \times e^{-\operatorname{tr}_{\mathcal{H}}((I_{\mathcal{H}} - A_0)^{-1}A_0A_1 z + O(z^2))} \\
&\underset{z\to 0}{=} \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)\det_{2,\mathcal{H}}\big(I_{\mathcal{H}} - (I_{\mathcal{H}} - A_0)^{-1}A_0A_1 z + O\big(z^2\big)\big) \\
&\quad \times \big[1 - \operatorname{tr}_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)^{-1}A_0A_1\big)z + O\big(z^2\big)\big] \\
&\underset{z\to 0}{=} \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0) \\
&\quad - \det_{2,\mathcal{H}}(I_{\mathcal{H}} - A_0)\operatorname{tr}_{\mathcal{H}}\big((I_{\mathcal{H}} - A_0)^{-1}A_0A_1\big)z + O\big(z^2\big).
\end{aligned} \tag{2.48}
$$

Here we used (cf. (2.43))

$$
\det_{2,\mathcal{H}}(I_{\mathcal{H}} - B(z)z) \underset{z\to 0}{=} 1 + O\big(z^2\big) \tag{2.49}
$$

for $B(\,\cdot\,)$ analytic in $\mathcal{B}_2(\mathcal{H})$-norm near $z = 0$. ☐

In exactly the same manner one obtains the Hilbert–Schmidt operator version of Theorem 2.3. Again we rely on the notation introduced in the paragraph preceding Theorem 2.3.

**Theorem 2.7.** *Assume Hypothesis* 2.5 *and let* $1 \in \sigma_{\mathrm{d}}(A_0)$. *Then,*

$$
\begin{aligned}
\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A(z)) &\underset{z\to 0}{=} \big[\det_{2,Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) + O(z)\big]e^{n_0} \\
&\qquad \times (-1)^{n_0}\det_{P_0\mathcal{H}}(P_0D_0P_0 + P_0[A_1 + O(z)]P_0 z) \qquad (2.50)\\
&\underset{z\to 0}{=} \det_{2,Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0)e^{n_0}\det_{\mathbb{C}^{n_0-\nu_0}}\big(\widetilde{A}_1\big)(-z)^{n_0-\nu_0} + O\big(z^{n_0-\nu_0+1}\big).
\end{aligned}
$$

*In the special case where* 1 *is a semisimple eigenvalue of* $A_0$ (*i.e., where* $D_0 = 0$ *and* $\nu_0 = 0$) *one obtains,*

$$
\begin{aligned}
\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A(z)) &\underset{z\to 0}{=} \det_{2,Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0)e^{n_0}\det_{P_0\mathcal{H}}(P_0A_1P_0)(-z)^{n_0} \\
&\qquad + O\big(z^{n_0+1}\big) \qquad (2.51)\\
&\underset{z\to 0}{=} \det_{2,\mathcal{H}}(I_{\mathcal{H}} - P_0 - A_0)e^{n_0}\det_{P_0\mathcal{H}}(P_0A_1P_0)z^{n_0} + O\big(z^{n_0+1}\big).
\end{aligned}
$$

*In particular, if* 1 *is a simple eigenvalue of* $A_0$ (*i.e., if* $n_0 = 1$, $D_0 = 0$, *and* $\nu_0 = 0$), *one obtains*

$$
\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A(z)) \underset{z\to 0}{=} \det_{2,\mathcal{H}}(I_{\mathcal{H}} - P_0 - A_0)\det_{P_0\mathcal{H}}(P_0A_1P_0)z + O\big(z^2\big). \tag{2.52}
$$

*Proof.* Again this follows from rewriting (2.26)–(2.28) in terms of modified Fredholm determinants $\det_{2,\mathcal{H}}(I_{\mathcal{H}} + \,\cdot\,)$, using (2.41),

$$\begin{aligned}
\operatorname{tr}_{\mathcal{H}}(A(z)) &= \operatorname{tr}_{\mathcal{H}}\big((P_0+Q_0)T(z)A(z)T(z)^{-1}(P_0+Q_0)\big)\\
&= \operatorname{tr}_{\mathcal{H}}\big(P_0T(z)A(z)T(z)^{-1}P_0\big) + \operatorname{tr}_{\mathcal{H}}\big(Q_0T(z)A(z)T(z)^{-1}Q_0\big)\\
&= \operatorname{tr}_{P_0\mathcal{H}}\big(P_0T(z)A(z)T(z)^{-1}P_0\big) + \operatorname{tr}_{Q_0\mathcal{H}}\big(Q_0T(z)A(z)T(z)^{-1}Q_0\big)\\
&\underset{z\to 0}{=} \operatorname{tr}_{P_0\mathcal{H}}(P_0A_0P_0) + O(z) + \operatorname{tr}_{Q_0\mathcal{H}}\big(Q_0T(z)A(z)T(z)^{-1}Q_0\big)\\
&\underset{z\to 0}{=} n_0 + O(z) + \operatorname{tr}_{Q_0\mathcal{H}}\big(Q_0T(z)A(z)T(z)^{-1}Q_0\big),
\end{aligned} \tag{2.53}$$

and then approximating Hilbert–Schmidt operators by trace class (or finite-rank) operators (cf., e.g., [17, Theorem III.7.1]). Here the fact that $\operatorname{tr}_{P_0\mathcal{H}}(P_0A_0P_0) = n_0$ follows from the canonical Jordan structure of $SP_0A_0P_0S^{-1}$ . Explicitly, one computes

$$\begin{aligned}
&\det_{2,\mathcal{H}}(I_{\mathcal{H}} - A(z)) = \det_{\mathcal{H}}(I_{\mathcal{H}} - A(z))e^{\operatorname{tr}_{\mathcal{H}}(A(z))}\\
&\quad = \det_{P_0\mathcal{H}}\big(I_{P_0\mathcal{H}} - P_0T(z)A(z)T(z)^{-1}P_0\big)\\
&\qquad \times \det_{2,Q_0\mathcal{H}}\big(I_{Q_0\mathcal{H}} - Q_0T(z)A(z)T(z)^{-1}Q_0\big)\\
&\qquad \times e^{-\operatorname{tr}_{Q_0\mathcal{H}}(Q_0T(z)A(z)T(z)^{-1}Q_0)}e^{\operatorname{tr}_{\mathcal{H}}(A(z))}\\
&\quad \underset{z\to 0}{=} \det_{P_0\mathcal{H}}\big(I_{P_0\mathcal{H}} - P_0T(z)A(z)T(z)^{-1}P_0\big)[\det_{2,Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) + O(z)]\\
&\qquad \times e^{n_0+O(z)}\\
&\quad \underset{z\to 0}{=} (-1)^{n_0}\det_{P_0\mathcal{H}}(P_0D_0P_0 + P_0[A_1+O(z)]P_0z))\\
&\qquad \times [\det_{2,Q_0\mathcal{H}}(I_{Q_0\mathcal{H}} - Q_0A_0Q_0) + O(z)]e^{n_0}.
\end{aligned} \tag{2.54}$$

□

2.3. **Higher modified determinants.** It is now obvious how to proceed in connection with higher modified Fredholm determinants $\det_p(\,\cdot\,)$, $p \in \mathbb{N}$, $n \geq 3$, when the family $A(\,\cdot\,)$ in Hypothesis 2.5 is replaced by one analytic near $z = 0$ in $\mathcal{B}_p(\mathcal{H})$-norm. We omit further details at this point.

## 3. One-Dimensional Reaction–Diffusion Equations and Schrödinger Operators with Nontrivial Spatial Asymptotics

As an elementary illustration of formula (2.28) and a view toward applications to reaction-diffusion equations, we now illustrate the abstract results of Section 2 in the context of one-dimensional Schrödinger operators. (For background literature on reaction-diffusion equations we refer, e.g., to [29], [33], [39].)

To motivate our considerations of one-dimensional Schrödinger operators in this section, we start with a brief discussion of a simple model for one-dimensional scalar reaction-diffusion equations of the type

$$w_t = w_{xx} + f(w),\ t > 0, \quad w(0) = w_0. \tag{3.1}$$

Here, we assume, for simplicity,

$$f \in C^1(\mathbb{R}),\ f, f' \in L^\infty(\mathbb{R}), \quad w_0 \in H^2(\mathbb{R}) \cap C^\infty(\mathbb{R}),\ w_0' \in H^2(\mathbb{R}), \tag{3.2}$$

with $w = w(x,t)$, $(x,t) \in \mathbb{R} \times [0,T]$, for some $T = T(w_0) > 0$, a mild solution of (3.1) satisfying $w \in C_b([0,T]; L^2(\mathbb{R}; dx))$.

As usual, $C_b([0,T];L^2(\mathbb{R};dx))$ denotes the space of bounded continuous maps from $[0,T]$ with values in $L^2(\mathbb{R};dx)$ and the sup norm

$$\|v\|_{C_b([0,T];L^2(\mathbb{R};dx))} = \sup_{s\in[0,T]} \|v(s)\|_{L^2(\mathbb{R};dx)}, \quad v \in C_b([0,T];L^2(\mathbb{R};dx)). \tag{3.3}$$

We refer, for instance, to [24] for more details in this context (see also, [19, Sect. 3.2]). Also, $H^m(\mathbb{R})$, $m \in \mathbb{N}$, denotes the standard Sobolev spaces of regular distributions which together with their derivatives up to the $m$th-order lie in $L^2(\mathbb{R};dx)$.

Assuming that $U$ is a stationary (steady state) solution of (3.1), that is, $U_t = 0$, and hence

$$U'' + f(U) = 0, \tag{3.4}$$

we now linearize (3.1) around $U$ and obtain the linearized problem,

$$v_t = Lv, \tag{3.5}$$

where $L$ in $L^2(\mathbb{R};dx)$ is given by

$$L = \frac{d^2}{dx^2} + f'(U), \quad \operatorname{dom}(L) = H^2(\mathbb{R}), \tag{3.6}$$

Since $U' \in H^2(\mathbb{R}) \cap C^\infty(\mathbb{R})$, one infers upon differentiating (3.4) with respect to $x$ that

$$L(U') = (U')'' + f'(U)U' = [U'' + f(U)]' = 0, \tag{3.7}$$

and hence, $0 \in \sigma_{\rm p}(L)$. Here $\sigma_{\rm p}(\,\cdot\,)$ abbreviates the point spectrum (i.e., the set of eigenvalues). Thus, the Schrödinger operator

$$H = -L = -\frac{d^2}{dx^2} - f'(U), \quad \operatorname{dom}(H) = H^2(\mathbb{R}), \tag{3.8}$$

in $L^2(\mathbb{R};dx)$ with the potential

$$V(x) = -f'(U(x)), \quad x \in \mathbb{R}, \tag{3.9}$$

has the special property of a zero eigenvalue, that is,

$$0 \in \sigma_{\rm p}(H), \tag{3.10}$$

and we will be studying the situation where in addition 0 is a discrete (and hence simple) eigenvalue of $H$ in great detail in the remainder of this section. In particular, under appropriate assumptions on the the "potential" term $-f'(U)$ in $H$, the Birman–Schwinger-type integral operator $K(z)$ associated with $H$ and the complex eigenvalue parameter $z \in \mathbb{C}$ will be a trace class operator with $K(0)$ having the eigenvalue 1. Consequently, the behavior of $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - K(z))$ for $z$ in a sufficiently small open neighborhood of $z = 0$, which determines linear stability of (3.1) around its stationary solution $U$ (cf. [19, Sect. 5.1, Ex. 6, Sect. 6.2], [25, Sects. 9.1.4, 9.1.5]), can be determined in accordance with Theorem 2.3 or alternatively, directly from Jost (respectively, Evans) function considerations, as discussed in Remark 3.5.

We conclude these illustrations with the following elementary example:

**Example 3.1.** *Let $n \in \mathbb{N}$, $n \geq 2$, $c > 0$, $\kappa > 0$, $x \in \mathbb{R}$, and consider*

$$f_n(w) = -(n-1)^2\kappa^2 w + (n-1)n\kappa^2 c^{-2/(n-1)} w^{(n+1)/(n-1)}, \tag{3.11}$$

$$U_n(x) = c[\cosh(\kappa x)]^{-n+1}. \tag{3.12}$$

*Then the potential* $V_n(x) = -f'(U_n(x))$ *in the corresponding Schrödinger operator* $H_n = -(d^2/dx^2) + V_n$ *coincides with a particular family of* $n$*-soliton Korteweg–de Vries (KdV) potentials*

$$V_n(x) = -f'(U_n(x)) = (n-1)^2\kappa^2 - n(n+1)\kappa^2[\cosh(\kappa x)]^{-2}, \tag{3.13}$$

$$\lim_{x\to\pm\infty} V_n(x) = (n-1)^2\kappa^2 > 0, \tag{3.14}$$

*and the zero-energy eigenfunction* $U_n'$ *satisfying* $H_n(U_n') = 0$ *is given by*

$$U_n'(x) = -(n-1)\kappa c \sinh(\kappa x)[\cosh(\kappa x)]^{-n}. \tag{3.15}$$

It seems a curious coincidence that $V_n$ should coincide with a particular family of $n$-soliton KdV potentials (there are many other such $n$-soliton KdV potentials, cf., e.g., [10, Example 1.31]) in this reaction-diffusion equation context.

Motivated by these considerations, we now start to investigate one-dimensional Schrödinger operators with a scalar potential displaying a nonzero asymptotics as $|x| \to \infty$.

**Hypothesis 3.2.** *Assume* $V\colon \mathbb{R} \to \mathbb{R}$ *is Lebesgue measurable and satisfies*

$$\int_{\mathbb{R}} dx\, |V(x) - V_\infty| < \infty \ \textit{ for some } \ V_\infty > 0. \tag{3.16}$$

Assuming Hypothesis 3.2 we introduce

$$W(x) = V(x) - V_\infty, \tag{3.17}$$

$$W(x) = v(x)u(x), \quad u(x) = \operatorname{sgn}(W(x))v(x), \ \ v(x) = |W(x)|^{1/2}, \tag{3.18}$$

for a.e. $x \in \mathbb{R}$, and define $H$ to be the (maximally defined) self-adjoint realization in $L^2(\mathbb{R}; dx)$ of the differential expression $\tau = -(d^2/dx^2) + V(x)$, $x \in \mathbb{R}$, obtained by the method of quadratic forms, or equivalently, by using the limit point theory for self-adjoint 2nd order ordinary differential operators,

$$Hf = \tau f, \tag{3.19}$$

$$f \in \operatorname{dom}(H) = \big\{ g \in L^2(\mathbb{R}; dx) \,\big|\, g, g' \in AC_{\rm loc}(\mathbb{R}); \tau g \in L^2(\mathbb{R}; dx) \big\}. \tag{3.20}$$

(Here $'$ denotes differentiation with respect to $x \in \mathbb{R}$.) This also implies

$$\operatorname{dom}\big(H^{1/2}\big) = H^1(\mathbb{R}). \tag{3.21}$$

We also introduce the self-adjoint operator $H^{(0)}$ in $L^2(\mathbb{R}; dx)$ associated with the differential expression $\tau^{(0)} = -(d^2/dx^2) + V_\infty$, $x \in \mathbb{R}$, replacing $V(\,\cdot\,)$ by its asymptotic value $V_\infty$ (in the sense of (3.16)),

$$H^{(0)} f = \tau^{(0)} f, \quad f \in \operatorname{dom}\big(H^{(0)}\big) = H^2(\mathbb{R}). \tag{3.22}$$

By well-known results, (3.16) implies

$$\sigma_{\rm ess}(H) = \sigma_{\rm ess}\big(H^{(0)}\big) = [V_\infty, \infty), \quad \sigma_{\rm d}(H) \subset (-\infty, V_\infty), \tag{3.23}$$

where $\sigma_{\rm ess}(\,\cdot\,)$ and $\sigma_{\rm d}(\,\cdot\,)$ denote the essential and discrete spectrum, respectively.

Applying the Birman–Schwinger principle (cf., e.g., [12, Sect. 3]),

$$H\Psi(\lambda_j) = \lambda_j \Psi(\lambda_j), \quad \lambda_j < V_\infty, \ \lambda_j \in \sigma_{\rm d}(H), \ \Psi(\lambda_j) \in \operatorname{dom}(H), \tag{3.24}$$

is equivalent to

$$K(\lambda_j)\Phi(\lambda_j) = \Phi(\lambda_j), \quad \lambda_j < V_\infty, \ \Phi(\lambda_j) \in L^2(\mathbb{R}; dx), \tag{3.25}$$

with equal finite geometric multiplicity of either eigenvalue problem (3.24) and (3.25). In particular, in this special one-dimensional context, the eigenvalue $\lambda_j$ of $H$ as well as the eigenvalue 1 of $K(\lambda_j)$ are necessarily simple. Here we abbreviated

$$K(z) = -\overline{u\big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1}v}, \quad z \in \mathbb{C}\backslash[V_\infty, \infty), \tag{3.26}$$

with $\overline{T}$ denoting the operator closure of $T$. We recall that the integral kernel $\big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1}(x,x')$ of the resolvent of $H^{(0)}$ is explicitly given by

$$\begin{aligned} \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1}(x,x') &= (i/2)(z-V_\infty)^{-1/2}e^{i(z-V_\infty)^{1/2}|x-x'|}, \\ z \in \mathbb{C}\backslash[V_\infty,\infty), \ \operatorname{Im}&\big((z-V_\infty)^{1/2}\big) > 0, \quad x, x' \in \mathbb{R}, \end{aligned} \tag{3.27}$$

and hence

$$K(z) \in \mathcal{B}_1\big(L^2(\mathbb{R};dx)\big), \quad z \in \mathbb{C}\backslash[V_\infty,\infty), \tag{3.28}$$

since $K(z)$ is the product of the two Hilbert–Schmidt operators (cf. [38, Ch. 4])

$$u\big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1/2} \text{ and } \overline{\big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1/2}v} \tag{3.29}$$

(no operator closure necessary in the first factor). In addition, $\Psi(\lambda_j)$ and $\Phi(\lambda_j)$ are related by

$$\Phi(\lambda_j, x) = u(x)\Psi(\lambda_j, x), \quad x \in \mathbb{R}, \tag{3.30}$$

and we note that $\Psi(\lambda_j, \cdot\,)$ is also bounded,

$$\Psi(\lambda_j, \cdot\,) \in L^\infty(\mathbb{R}) \tag{3.31}$$

(in fact, even exponentially decaying with respect to $x$ by standard iterations of the Volterra integral equations (3.43)). Here the discrete eigenvalues $\sigma_{\rm d}(H) = \{\lambda_j\}_{j\in J}$ of $H$, with $J \subseteq \mathbb{N}$ an appropriate (finite or infinite) index set, are ordered as follows:

$$\lambda_1 < \lambda_2 < \cdots < V_\infty. \tag{3.32}$$

Moreover, one obtains

$$K(\overline{z})^* = -\overline{v\big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1}u}, \quad z \in \mathbb{C}\backslash[V_\infty,\infty), \tag{3.33}$$

and hence

$$K(\overline{z})^* = SK(z)S^{-1}, \quad z \in \mathbb{C}\backslash[V_\infty,\infty), \tag{3.34}$$

where $S$ denotes the unitary operator of multiplication by $\operatorname{sgn}(W(\cdot\,))$ in $L^2(\mathbb{R};dx)$,

$$(Sf)(x) = \operatorname{sgn}(W(x))f(x) \text{ for a.e. } x \in \mathbb{R}, \ f \in L^2(\mathbb{R};dx). \tag{3.35}$$

Thus,

$$K(\lambda_j)^*\widetilde{\Phi}(\lambda_j) = \widetilde{\Phi}(\lambda_j), \quad \lambda_j < V_\infty, \ \widetilde{\Phi}(\lambda_j) \in L^2(\mathbb{R};dx), \tag{3.36}$$

where

$$\widetilde{\Phi}(\lambda_j, x) = C(\lambda_j)(S\Phi(\lambda_j))(x) = C(\lambda_j)v(x)\Psi(\lambda_j,x) \text{ for some } C(\lambda_j) \in \mathbb{C}\backslash\{0\}. \tag{3.37}$$

To fix the normalization constant $C(\lambda_j)$ we require

$$\big(\widetilde{\Phi}(\lambda_j), \Phi(\lambda_j)\big)_{L^2(\mathbb{R};dx)} = 1. \tag{3.38}$$

This yields

$$C(\lambda_j) = \bigg[\int_{\mathbb{R}} dx\, W(x)|\Psi(\lambda_j,x)|^2\bigg]^{-1} = (v\Psi(\lambda_j), u\Psi(\lambda_j))^{-1}_{L^2(\mathbb{R};dx)} \tag{3.39}$$

and hence

$$\widetilde{\Phi}(\lambda_j,x) = \bigg[\int_{\mathbb{R}} dx\, W(x)|\Psi(\lambda_j,x)|^2\bigg]^{-1} \operatorname{sgn}(W(x))\Phi(\lambda_j,x) \tag{3.40}$$

$$= \bigg[\int_{\mathbb{R}} dx\, W(x)|\Psi(\lambda_j,x)|^2\bigg]^{-1} v(x)\Psi(\lambda_j,x). \tag{3.41}$$

In particular, the corresponding one-dimensional Riesz projection $P(\lambda_j)$ onto the eigenspace corresponding to the eigenvalue 1 of $K(\lambda_j)$ is then of the simple form

$$P(\lambda_j) = \big(\widetilde{\Phi}(\lambda_j),\,\cdot\,\big)_{L^2(\mathbb{R};dx)}\Phi(\lambda_j), \quad \lambda_j < V_\infty. \tag{3.42}$$

3.1. **The Jost–Pais derivative formula.** Next, consider the generalized Jost-type (distributional) solutions

$$\begin{aligned}\Psi_\pm(z,x) &= e^{\pm i(z-V_\infty)^{1/2}x} \\ &\quad - \int_x^{\pm\infty} dx'\, \frac{\sin((z-V_\infty)^{1/2}(x-x'))}{(z-V_\infty)^{1/2}}[V(x')-V_\infty]\Psi_\pm(z,x'), \\ &\qquad z\in\mathbb{C}\backslash[V_\infty,\infty),\ \operatorname{Im}\big((z-V_\infty)^{1/2}\big)>0,\ x\in\mathbb{R},\end{aligned} \tag{3.43}$$

of $L\Psi(z) = z\Psi(z)$. Then,

$$\Psi_\pm(\lambda,x) \text{ are real-valued for } \lambda<V_\infty,\ x\in\mathbb{R}, \tag{3.44}$$

and

$$\Psi_\pm(\lambda,x)>0 \text{ for } \lambda<V_\infty \text{ and } \pm x \text{ sufficiently large.} \tag{3.45}$$

The Jost function $\mathcal{F}$ associated with $H$ is then given by

$$\mathcal{F}(z) = \frac{\operatorname{Wr}(\Psi_-(z),\Psi_+(z))}{2i(z-V_\infty)^{1/2}} \tag{3.46}$$

$$= 1 + \frac{i}{2(z-V_\infty)^{1/2}}\int_{\mathbb{R}} dx\, e^{\mp i(z-V_\infty)^{1/2}x}[V(x)-V_\infty]\Psi_\pm(z,x), \quad z\in\mathbb{C}\backslash[V_\infty,\infty), \tag{3.47}$$

where $\operatorname{Wr}(f,g)(x) = f(x)g'(x) - f'(x)g(x)$, $x\in\mathbb{R}$, $f,g\in C^1(\mathbb{R})$, denotes the Wronskian of $f$ and $g$. The limits to the real axis

$$\lim_{\varepsilon\downarrow 0}\mathcal{F}(\lambda\pm i\varepsilon) = \mathcal{F}(\lambda\pm i0) \tag{3.48}$$

exist and are continuous for all $\lambda\in\mathbb{R}\backslash\{V_\infty\}$. In addition, one verifies

$$\mathcal{F}(z) \underset{|z|\to\infty}{\longrightarrow} 1. \tag{3.49}$$

Moreover, one can prove the following result originally due to Jost and Pais [20] (for $V_\infty = 0$) in the context of half-line Schrödinger operators. The actual case at hand of Schrödinger operators on the whole real line (again for $V_\infty = 0$) was discussed by Newton [26] and we refer to [13] for more background and details,

$$\mathcal{F}(z) = {\det}_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - K(z)), \quad z\in\mathbb{C}\backslash[V_\infty,\infty). \tag{3.50}$$

Since we are interested especially in the $z$-derivative of $\mathcal{F}(z)$ at a discrete eigenvalue of $H$, we now prove the following result, Lemma 3.3. For the remainder of this paper we abbreviate differentiation with respect to the complex-valued spectral parameter $z\in\mathbb{C}$ by $\bullet$ (to distinguish it from differentiation with respect to the space variable $x\in\mathbb{R}$).

**Lemma 3.3.** *Assume Hypothesis* 3.2 *and* $z \in \mathbb{C}\backslash[V_\infty, \infty)$. *Moreover, let* $\lambda_j < V_\infty$, $\lambda_j \in \sigma_{\rm d}(H)$. *Then,* $\mathcal{F}(\lambda_j) = 0$ *and*

$$\mathcal{F}^\bullet(\lambda_j) = \frac{-1}{2(V_\infty - \lambda_j)^{1/2}} \int_{\mathbb{R}} dx\, \Psi_-(\lambda_j, x)\Psi_+(\lambda_j, x). \tag{3.51}$$

*Proof.* Consider

$$\Psi''_\pm(z,x) = [V(x)-z]\Psi_\pm(z,x), \quad \Psi^{\bullet\prime\prime}_\pm(z,x) = [V(x)-z]\Psi^\bullet_\pm(z,x) - \Psi_\pm(z,x) \tag{3.52}$$

(we recall that $\bullet$ abbreviates $d/dz$) to derive the identities

$$\frac{d}{dx}\text{Wr}(\Psi_-(z,x), \Psi^\bullet_+(z,x)) = -\Psi_-(z,x)\Psi_+(z,x), \tag{3.53}$$

$$\frac{d}{dx}\text{Wr}(\Psi^\bullet_-(z,x), \Psi_+(z,x)) = \Psi_-(z,x)\Psi_+(z,x). \tag{3.54}$$

Then one obtains for all $R > 0$,

$$\begin{aligned}
&\text{Wr}(\Psi_-(z), \Psi^\bullet_+(z))(x) + \text{Wr}(\Psi^\bullet_-(z), \Psi_+(z))(x) \\
&\quad - \text{Wr}(\Psi_-(z), \Psi^\bullet_+(z))(R) - \text{Wr}(\Psi^\bullet_-(z), \Psi_+(z))(-R) \\
&= -\int_x^R dx'\, \frac{d}{dx'}\text{Wr}(\Psi_-(z,x'), \Psi^\bullet_+(z,x')) + \int_{-R}^x dx'\, \frac{d}{dx'}\text{Wr}(\Psi^\bullet_-(z,x'), \Psi_+(z,x')) \\
&= \int_{-R}^R dx'\, \Psi_-(z,x')\Psi_+(z,x').
\end{aligned} \tag{3.55}$$

Next, we note that

$$\frac{d}{dz}\text{Wr}(\Psi_-(z), \Psi_+(z)) = \text{Wr}(\Psi_-(z), \Psi^\bullet_+(z)) + \text{Wr}(\Psi^\bullet_-(z), \Psi_+(z)), \tag{3.56}$$

and choosing $z = \lambda_j < V_\infty$, $\lambda_j \in \sigma_{\rm d}(H)$, one concludes $\Psi_\pm(\lambda_j, \cdot\,) \in L^2(\mathbb{R}; dx)$ and hence,

$$\frac{d}{dz}\text{Wr}(\Psi_-(z), \Psi_+(z))\big|_{z=\lambda_j} = \int_{\mathbb{R}} dx\, \Psi_-(\lambda_j, x)\Psi_+(\lambda_j, x). \tag{3.57}$$

Together with (3.46) and

$$2i(\lambda_j - V_\infty)^{1/2}\mathcal{F}(\lambda_j) = \text{Wr}(\Psi_-(\lambda_j), \Psi_+(\lambda_j)) = 0, \tag{3.58}$$

this establishes (3.51). □

Next, we specialize to the case $\lambda_j = 0$ and hence assume

$$0 \in \sigma_{\rm d}(H). \tag{3.59}$$

In this context we then denote

$$\Psi_0 = \Psi(0),\ \Phi_0 = \Phi(0),\ \widetilde{\Phi}_0 = \widetilde{\Phi}(0),\ C_0 = C(0),\ K_0 = K(0),\ P_0 = P(0),\ \text{etc.}, \tag{3.60}$$

and without loss of generality (cf. (3.44)) we assume that $\Psi_0(x)$ is real-valued for all $x \in \mathbb{R}$.

We summarize the results for $\mathcal{F}^\bullet(0)$:

**Lemma 3.4.** *Assume Hypothesis* 3.2 *and suppose* $0 \in \sigma_{\rm d}(H)$. *Then,* $\mathcal{F}(0) = 0$ *and*

$$\mathcal{F}^\bullet(0) = \frac{-1}{2V_\infty^{1/2}} \int_{\mathbb{R}} dx\, \Psi_-(0,x)\Psi_+(0,x) \tag{3.61}$$

$$= \begin{cases} < 0 & \text{if } \Psi_\pm(0,\,\cdot\,) \text{ has an even number of zeros on } \mathbb{R}, \\ > 0 & \text{if } \Psi_\pm(0,\,\cdot\,) \text{ has an odd number of zeros on } \mathbb{R}, \end{cases} \tag{3.62}$$

$$= \begin{cases} < 0 & \text{if } 0 \text{ is an odd eigenvalue of } H, \\ > 0 & \text{if } 0 \text{ is an even eigenvalue of } H. \end{cases} \tag{3.63}$$

*Here the eigenvalues* $\{\lambda_j\}_{j\in J}$, $J \subseteq \mathbb{N}$ *an appropriate (finite or infinite) index set, are ordered in magnitude according to* $\lambda_1 < \lambda_2 < \cdots < V_\infty$ *(cf.* (3.32)*).*

*Proof.* Equation (3.62) is immediate from (3.45) and $\Psi_+(0,x) = c\Psi_-(0,x)$ for some $c \in \mathbb{R}\backslash\{0\}$ (cf. (3.97)). Relation (3.63) is a direct consequence of the fact that $H$ is bounded from below, $H \geq \lambda_1 I_{L^2(\mathbb{R};dx)}$, the discrete eigenvalues of $H$ are in a one-to-one correspondence with the zeros of $\mathcal{F}$ on $[\lambda_1, V_\infty)$ (the zeros necessarily being all simple), and the fact that $\mathcal{F}(z) \underset{|z|\to\infty}{\longrightarrow} 1$, $z \in \mathbb{C}\backslash[V_\infty,\infty)$ (cf. (3.49)). ☐

**Remark 3.5.** Since $\mathcal{F}(\lambda \pm i0) \underset{\lambda\to\pm\infty}{\longrightarrow} 1$ by (3.49), $\mathcal{F}(0) = 0$ and $\mathcal{F}^\bullet(0) > 0$ imply that $H$ has at least one negative eigenvalue and hence $L = -H$ (cf. (3.8)) has at least one positive eigenvalue. This implies linear instability of the stationary solution $U$ in the context of the reaction-diffusion equation (3.1) identifying $V(x)$ and $-f'(U(x))$, $x \in \mathbb{R}$ (cf. (3.9)). For, it is easily seen by consideration of the standing-wave equation (3.4), a scalar nonlinear oscillator, that the derivative $U'$ of a pulse-type solution has precisely one zero, whereas $\Psi_\pm$ are nonzero multiples of the zero eigenfunction $U'$. For discussion of spectral stability and some of its applications, we refer, for instance, to [30], [31], [35], [47], [48], and the references cited therein. An equivalent formula for $\mathcal{F}^\bullet$ yielding the same conclusions may be derived in straightforward fashion by Evans function techniques, following the standard approach introduced in [6], [7], [8], [9]. We recall (cf. [11]) that Jost and Evans functions, suitably normalized, agree.

3.2. **Fredholm determinant version.** We now turn to the connection with the abstract approach to the asymptotic behavior of Fredholm determinants presented in Section 2.

Applying (2.28) to (3.50) one then obtains

$$\mathcal{F}^\bullet(0) = \det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - K_0 - P_0)\det_{P_0L^2(\mathbb{R};dx)}(P_0K_1P_0), \tag{3.64}$$

where

$$K(z) \underset{z\to 0}{=} K_0 + K_1 z + O\big(z^2\big) \tag{3.65}$$

with

$$K_0 = -\overline{uH^{(0)^{-1}}}v, \tag{3.66}$$

$$K_1 = K^\bullet(z)\big|_{z=0} = -\overline{uH^{(0)^{-2}}}v. \tag{3.67}$$

3.2.1. *Evaluation of the second factor.* We start by determining the second factor $\det_{P_0L^2(\mathbb{R};dx)}(P_0K_1P_0)$ on the right-hand side of (3.64):

**Theorem 3.6.** *Assume Hypothesis* 3.2 *and suppose* $0 \in \sigma_{\rm d}(H)$*. Then,*

$$\det_{P_0L^2(\mathbb{R};dx)}(P_0K_1P_0) = -\|\Psi_0\|^2_{L^2(\mathbb{R};dx)}\big/(v\Psi_0, u\Psi_0)_{L^2(\mathbb{R};dx)} \tag{3.68}$$

$$= \big[\|\Psi_0'\|^2_{L^2(\mathbb{R};dx)} + V_\infty\|\Psi_0\|^2_{L^2(\mathbb{R};dx)}\big]^{-1}\|\Psi_0\|^2_{L^2(\mathbb{R};dx)} > 0. \tag{3.69}$$

*Proof.* First, we choose a compactly supported sequence $W_n \in C_0^\infty(\mathbb{R})$, $n \in \mathbb{N}$, such that

$$W_n = V_n - V_\infty = u_n v_n, \quad u_n = \operatorname{sgn}(W_n) v_n, \ \ v_n = |W_n|^{1/2}, \ n \in \mathbb{N}, \tag{3.70}$$

and

$$\lim_{n\to\infty} \|v_n - v\|_{L^2(\mathbb{R};dx)} = 0. \tag{3.71}$$

Given $W_n$, we introduce the self-adjoint operator sum $H_n = H^{(0)} + W_n$ in $L^2(\mathbb{R};dx)$ defined on the domain $H^2(\mathbb{R})$ associated with the differential expression $L_n = -(d^2/dx^2) + V_n(x)$, $x \in \mathbb{R}$, $n \in \mathbb{N}$. Then $H_n$ converges to $H$ in norm resolvent sense as $n \to \infty$, that is,

$$\lim_{n\to\infty} \big\| \big(H_n - zI_{L^2(\mathbb{R};dx)}\big)^{-1} - \big(H - zI_{L^2(\mathbb{R};dx)}\big)^{-1} \big\| = 0, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.72}$$

This follows from the resolvent identities,

$$\begin{aligned} &\big(H_n - zI_{L^2(\mathbb{R};dx)}\big)^{-1} = \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1} \\ &\quad - \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1} v_n \big[I_{L^2(\mathbb{R};dx)} - K_n(z)\big]^{-1} u_n \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1}, \\ &\hspace{20em} z \in \mathbb{C}\backslash\sigma(H_n), \end{aligned} \tag{3.73}$$

$$\begin{aligned} &\big(H - zI_{L^2(\mathbb{R};dx)}\big)^{-1} = \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1} \\ &\quad - \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1} v \big[I_{L^2(\mathbb{R};dx)} - K(z)\big]^{-1} u \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1}, \\ &\hspace{20em} z \in \mathbb{C}\backslash\sigma(H), \end{aligned} \tag{3.74}$$

where

$$K_n(z) = u_n \big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1} v_n, \quad z \in \mathbb{C}\backslash\sigma\big(H^{(0)}\big), \ n \in \mathbb{N}, \tag{3.75}$$

and $K(z)$ is given by (3.26), and the fact that (3.71) implies

$$\lim_{n\to\infty} \big\|(v_n - v)\big(H^{(0)} - zI_{L^2(\mathbb{R};dx)}\big)^{-1/2}\big\|_{\mathcal{B}_2(L^2(\mathbb{R};dx))} = 0, \quad z \in \mathbb{C}\backslash\sigma\big(H^{(0)}\big) \tag{3.76}$$

(cf. the detailed discussion in [13]). Thus, the spectrum of $H_n$ converges to that of $H$ as $n \to \infty$. In particular, for $n \in \mathbb{N}$ sufficiently large, $H_n$ has a simple eigenvalue $\lambda_n$ in a small neighborhood of $z = 0$ satisfying

$$\lambda_n \underset{n\to\infty}{\longrightarrow} 0. \tag{3.77}$$

We denote by $\Psi_n$ the corresponding eigenfunction of $H_n$, associated with the eigenvalue $\lambda_n$ of $H_n$, $H_n\Psi_n = \lambda_n\Psi_n$, $n \in \mathbb{N}$. $\Psi_n$ is then a constant multiple of the solutions satisfying (3.43) with $z = \lambda_n$ and $V$ replaced by $V_n$. We may choose the constant multiple in $\Psi_n$ such that

$$\lim_{n\to\infty} \|\Psi_n - \Psi_0\|_{L^2(\mathbb{R};dx)} = 0. \tag{3.78}$$

In addition, we recall that (3.43) also implies that $\Psi_n$ and $\Psi_0$ are exponentially bounded in $x \in \mathbb{R}$ with bounds uniform with respect to $n \in \mathbb{N}$.

In addition, we abbreviate

$$\Phi_n = u_n\Psi_n, \quad \widetilde{\Phi}_n = C_n S_n \Phi_n, \quad \big(\widetilde{\Phi}_n, \Phi_n\big)_{L^2(\mathbb{R};dx)} = 1, \tag{3.79}$$

$$P_n = \big(\widetilde{\Phi}_n, \cdot\,\big)\Phi_n, \tag{3.80}$$

$$S_n f = \operatorname{sgn}(W_n) f, \quad f \in L^2(\mathbb{R};dx), \tag{3.81}$$

$$C_n = \bigg[\int_{\mathbb{R}} dx\, W_n(x)|\Psi_n(x)|^2\bigg]^{-1}, \tag{3.82}$$

$$K_n(z) \underset{z\to\lambda_n}{=} K_{0,n} + K_{1,n}(z-\lambda_n) + O\big((z-\lambda_n)^2\big), \tag{3.83}$$

$$K_{0,n} = -u_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}v_n, \quad K_{1,n} = -u_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-2}v_n, \quad n\in\mathbb{N}, \tag{3.84}$$

and recall that

$$-u_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}v_n\Phi_n = \Phi_n, \quad -v_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}u_n\widetilde{\Phi}_n = \widetilde{\Phi}_n, \tag{3.85}$$

$$H_n\Psi_n = \big(H^{(0)} + W_n\big)\Psi_n = \lambda_n\Psi_n, \quad -\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}W_n\Psi_n = \Psi_n, \ n\in\mathbb{N}. \tag{3.86}$$

We note that since $u_n, v_n, W_n$, $n\in\mathbb{N}$, are all bounded operators on $L^2(\mathbb{R};dx)$, no operator closure symbols in $u_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-k}v_n$, $k=1,2$, are needed in the following computation leading up to (3.87).

Next, one computes

$$\begin{aligned}
&\det{}_{P_nL^2(\mathbb{R};dx)}(P_nK_{1,n}P_n) = -\det{}_{P_nL^2(\mathbb{R};dx)}\big(P_nu_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-2}v_nP_n\big) \\
&\quad = -\big(\widetilde{\Phi}_n, u_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-2}v_n\Phi_n\big)_{L^2(\mathbb{R};dx)} \\
&\quad = -\big(\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}u_n\widetilde{\Phi}_n, \big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}v_n\Phi_n\big)_{L^2(\mathbb{R};dx)} \\
&\quad = -C_n\big(\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}W_n\Psi_n, \big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-1}W_n\Psi_n\big)_{L^2(\mathbb{R};dx)} \\
&\quad = -C_n\big\|\Psi_n\big\|^2_{L^2(\mathbb{R};dx)}, \quad n\in\mathbb{N}.
\end{aligned} \tag{3.87}$$

Since

$$\lim_{n\to\infty} C_n = C_0 = \bigg[\int_{\mathbb{R}} dx\, W(x)|\Psi_0(x)|^2\bigg]^{-1}, \tag{3.88}$$

one finally obtains,

$$\begin{aligned}
\det{}_{P_0L^2(\mathbb{R};dx)}(P_0K_1P_0) &= -\det{}_{P_0L^2(\mathbb{R};dx)}\Big(P_0\overline{uH^{(0)}{}^{-2}v}P_0\Big) \\
&= -\Big(\widetilde{\Phi}_0, \overline{uH^{(0)}{}^{-2}v}\Phi_0\Big)_{L^2(\mathbb{R};dx)} \\
&= -\lim_{n\to\infty}\big(\widetilde{\Phi}_n, u_n\big(H^{(0)} - \lambda_n I_{L^2(\mathbb{R};dx)}\big)^{-2}v_n\Phi_n\big)_{L^2(\mathbb{R};dx)} \\
&= -\lim_{n\to\infty} C_n\big\|\Psi_n\big\|^2_{L^2(\mathbb{R};dx)} \\
&= -C_0\|\Psi_0\|^2_{L^2(\mathbb{R};dx)} \qquad (3.89) \\
&= -\bigg[\int_{\mathbb{R}} dx\, W(x)|\Psi_0(x)|^2\bigg]^{-1}\|\Psi_0\|^2_{L^2(\mathbb{R};dx)} \qquad (3.90) \\
&= -\|\Psi_0\|^2_{L^2(\mathbb{R};dx)}/(v\Psi_0, u\Psi_0)_{L^2(\mathbb{R};dx)} \qquad (3.91) \\
&= \big[\|\Psi_0'\|^2_{L^2(\mathbb{R};dx)} + V_\infty\|\Psi_0\|^2_{L^2(\mathbb{R};dx)}\big]^{-1}\|\Psi_0\|^2_{L^2(\mathbb{R};dx)} > 0. \qquad (3.92)
\end{aligned}$$

Here we applied the quadratic form equality

$$\begin{aligned} 0 &< \|\Psi_0'\|^2_{L^2(\mathbb{R};dx)} + V_\infty \|\Psi_0\|^2_{L^2(\mathbb{R};dx)} = -(v\Psi_0, u\Psi_0)_{L^2(\mathbb{R};dx)} \\ &= -\int_{\mathbb{R}} dx\, W(x)|\Psi_0(x)|^2 \end{aligned} \tag{3.93}$$

to (3.90), to arrive at (3.92). □

3.2.2. *The first factor: A posteriori computation.* Before we proceed to a direct approach to compute the first factor on the right-hand side of (3.64),

$$\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - K_0 - P_0), \tag{3.94}$$

we will next determine $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - K_0 - P_0)$ by using the final answer (3.51) for $\mathcal{F}^\bullet(0)$.

**Theorem 3.7.** *Assume Hypothesis* 3.2 *and suppose* $0 \in \sigma_{\rm d}(H)$. *Then,*

$$\begin{aligned} &\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0) \\ &\quad = \frac{1}{2V_\infty^{1/2}} \int_{\mathbb{R}} dx\, [V(x) - V_\infty]\Psi_+(0,x)\Psi_-(0,x) \qquad (3.95)\\ &\quad = -\big[2V_\infty^{1/2}\big]^{-1} \|\Psi_\pm(0)\|^{-2}_{L^2(\mathbb{R};dx)} \big[\|\Psi_\pm'(0)\|^2_{L^2(\mathbb{R};dx)} + V_\infty\|\Psi_\pm(0)\|^2_{L^2(\mathbb{R};dx)}\big] \\ &\qquad \times (\Psi_-(0), \Psi_+(0))_{L^2(\mathbb{R};dx)}. \qquad (3.96) \end{aligned}$$

(*Here the equations for the* + *and* − *sign should be read separately.*)

*Proof.* Combining (3.44), (3.51) (setting $\lambda_j = 0$), (3.64), (3.68), and (3.89), and taking into account that for some constants $C_\pm \in \mathbb{R}\backslash\{0\}$,

$$\Psi_0(x) = C_\pm \Psi_\pm(0,x), \quad x \in \mathbb{R}, \tag{3.97}$$

then yields for the first factor in (3.64),

$$\begin{aligned} &\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0) = \frac{\mathcal{F}^\bullet(0)}{\det_{P_0L^2(\mathbb{R};dx)}(P_0K_1P_0)} \\ &\quad = C_0^{-1}\|\Psi_0\|^{-2} \frac{1}{2V_\infty^{1/2}} \int_{\mathbb{R}} dx'\, \Psi_-(0,x')\Psi_+(0,x') \\ &\quad = \big[2V_\infty^{1/2}\big]^{-1} \|\Psi_0\|^{-2}_{L^2(\mathbb{R};dx)} (v\Psi_0, u\Psi_0)_{L^2(\mathbb{R};dx)} (\Psi_-(0), \Psi_+(0))_{L^2(\mathbb{R};dx)} \\ &\quad = \big[2V_\infty^{1/2}\big]^{-1} \|\Psi_\pm(0)\|^{-2}_{L^2(\mathbb{R};dx)} (v\Psi_\pm(0), u\Psi_\pm(0))_{L^2(\mathbb{R};dx)} (\Psi_-(0), \Psi_+(0))_{L^2(\mathbb{R};dx)} \\ &\quad = \frac{1}{2V_\infty^{1/2}} \int_{\mathbb{R}} dx\, [V(z) - V_\infty]\Psi_+(0,x)\Psi_-(0,x) \\ &\quad = -\big[2V_\infty^{1/2}\big]^{-1} \|\Psi_\pm(0)\|^{-2}_{L^2(\mathbb{R};dx)} \big[\|\Psi_\pm'(0)\|^2_{L^2(\mathbb{R};dx)} + V_\infty\|\Psi_\pm(0)\|^2_{L^2(\mathbb{R};dx)}\big] \\ &\qquad \times (\Psi_-(0), \Psi_+(0))_{L^2(\mathbb{R};dx)}. \end{aligned} \tag{3.98}$$

□

3.2.3. *The first factor: Direct computation.* Next, we proceed to a direct approach to compute the first factor on the right-hand side of (3.64), $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - K_0 - P_0)$. This will now be an *ab initio* calculation entirely independent of the result (3.61).

**Theorem 3.8.** *Assume Hypothesis* 3.2 *and suppose* $0 \in \sigma_{\rm d}(H)$. *Then,*

$$\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0) = \frac{-1}{2V_\infty^{1/2}} \int_{\mathbb{R}} dx\, [V(x) - V_\infty] e^{\pm V_\infty^{1/2} x} \psi_\pm(x), \quad (3.99)$$

*where* $\psi_\pm$ *are defined by*

$$\psi_\pm(x) = -\Psi_\pm(0,x) - \frac{1}{V_\infty^{1/2}} \int_x^{\pm\infty} dx'\, \sinh\big(V_\infty^{1/2}(x-x')\big)[V(x') - V_\infty]\psi_\pm(x'), \quad x \in \mathbb{R}. \quad (3.100)$$

(*Here the equations for the* $+$ *and* $-$ *sign should be read separately.*)

*Proof.* Our strategy is to apply formulas (3.9) and (3.12) in [13] to the Fredholm determinant $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0)$ by appealing to the semi-separable nature of $P_0 + K_0$ upon an appropriate reformulation involving block operator matrices. To this end we introduce

$$f_1(x) = \Big(-u(x)e^{-V_\infty^{1/2}x} \quad u(x)\Psi_0(x)\Big), \quad (3.101)$$

$$g_1(x) = \Big([2(V_\infty)^{1/2}]^{-1} v(x) e^{V_\infty^{1/2}x} \quad C_0 v(x)\Psi_0(x)\Big)^\top, \quad (3.102)$$

$$f_2(x) = \Big(-u(x)e^{V_\infty^{1/2}x} \quad u(x)\Psi_0(x)\Big), \quad (3.103)$$

$$g_2(x) = \Big([2(V_\infty)^{1/2}]^{-1} v(x) e^{-V_\infty^{1/2}x} \quad C_0 v(x)\Psi_0(x)\Big)^\top \quad (3.104)$$

and note that $P_0 + K_0$ is an integral operator with semi-separable integral kernel

$$(P_0 + K_0)(x,x') = \begin{cases} f_1(x)g_1(x'), & x' < x, \\ f_2(x)g_2(x'), & x' > x. \end{cases} \quad (3.105)$$

In addition, we introduce the integral kernel

$$H(x,x') = f_1(x)g_1(x') - f_2(x)g_2(x') = u(x)\frac{\sinh\big(V_\infty^{1/2}(x-x')\big)}{V_\infty^{1/2}} v(x'), \quad (3.106)$$

and, temporarily assuming that

$$\operatorname{supp}(V - V_\infty) \text{ is compact}, \quad (3.107)$$

the pair of Volterra integral equations

$$\hat f_1(x) = f_1(x) - \int_x^\infty dx'\, H(x,x')\hat f_1(x'), \quad (3.108)$$

$$\hat f_2(x) = f_2(x) + \int_{-\infty}^x dx'\, H(x,x')\hat f_2(x') \quad (3.109)$$

for a.e. $x \in \mathbb{R}$. Applying Theorem 3.2 of [13] (especially, (3.9) and (3.12) in [13]) one then infers

$$\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0) = \det_{\mathbb{C}^2}\bigg(I_2 - \int_{\mathbb{R}} dx\, g_1(x)\hat f_1(x)\bigg) \quad (3.110)$$

$$= \det_{\mathbb{C}^2}\bigg(I_2 - \int_{\mathbb{R}} dx\, g_2(x)\hat f_2(x)\bigg), \quad (3.111)$$

with $I_2$ the identity matrix in $\mathbb{C}^2$. Introducing $\widehat{\Psi}_\pm$ as the solutions of the pair of Volterra integral equations

$$\begin{aligned}\widehat{\Psi}_\pm(x) &= \begin{pmatrix} e^{\mp V_\infty^{1/2}x} & -\Psi_0(x)\end{pmatrix} \\ &\quad - \frac{1}{V_\infty^{1/2}}\int_x^{\pm\infty} dx'\, \sinh\big(V_\infty^{1/2}(x-x')\big)[V(x')-V_\infty]\widehat{\Psi}_\pm(x'), \quad x\in\mathbb{R},\end{aligned} \tag{3.112}$$

a comparison with (3.108) and (3.109) yields

$$\hat f_1(x) = -u(x)\widehat{\Psi}_+(x),\ \hat f_2(x) = -u(x)\widehat{\Psi}_-(x) \text{ for a.e. } x\in\mathbb{R}. \tag{3.113}$$

Writing

$$\widehat{\Psi}_\pm(x) = \begin{pmatrix}\Psi_\pm(0,x) & \hat\psi_\pm(x)\end{pmatrix}, \quad x\in\mathbb{R}, \tag{3.114}$$

(3.112) yields ($x\in\mathbb{R}$)

$$\hat\psi_\pm(x) = -\Psi_0(x) - \frac{1}{V_\infty^{1/2}}\int_x^{\pm\infty} dx'\, \sinh\big(V_\infty^{1/2}(x-x')\big)[V(x')-V_\infty]\hat\psi_\pm(x'), \tag{3.115}$$

and

$$\Psi_\pm(0,x) = e^{\mp V_\infty^{1/2}x} - \frac{1}{V_\infty^{1/2}}\int_x^{\pm\infty} dx'\, \sinh\big(V_\infty^{1/2}(x-x')\big)[V(x')-V_\infty]\Psi_\pm(0,x'), \tag{3.116}$$

in accordance with (3.43) for $z=0$. Because of (3.97), $\Psi_0(x) = C_\pm\Psi_\pm(0,x)$, $x\in\mathbb{R}$, one infers that

$$\psi_\pm(x) = C_\pm^{-1}\hat\psi_\pm(x), \quad x\in\mathbb{R}, \tag{3.117}$$

with $\psi_\pm$ satisfying (3.100).

Next, one computes

$$g_1(x)\hat f_1(x) = \begin{pmatrix} -\frac{\exp\left(V_\infty^{1/2}x\right)}{2V_\infty^{1/2}}[V(x)-V_\infty]\Psi_+(0,x) & -\frac{\exp\left(V_\infty^{1/2}x\right)}{2V_\infty^{1/2}}[V(x)-V_\infty]\hat\psi_+(x) \\ -C_0[V(x)-V_\infty]\Psi_0(x)\Psi_+(0,x) & -C_0[V(x)-V_\infty]\Psi_0(x)\hat\psi_+(x)\end{pmatrix}, \tag{3.118}$$

$$g_2(x)\hat f_2(x) = \begin{pmatrix} -\frac{\exp\left(-V_\infty^{1/2}x\right)}{2V_\infty^{1/2}}[V(x)-V_\infty]\Psi_-(0,x) & -\frac{\exp\left(-V_\infty^{1/2}x\right)}{2V_\infty^{1/2}}[V(x)-V_\infty]\hat\psi_-(x) \\ -C_0[V(x)-V_\infty]\Psi_0(x)\Psi_-(0,x) & -C_0[V(x)-V_\infty]\Psi_0(x)\hat\psi_-(x)\end{pmatrix}. \tag{3.119}$$

Using the fact that $0\in\sigma_{\rm d}(H)$, and hence $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)}-K_0)=0$, one obtains from taking $z=0$ in (3.47) and (3.50),

$$\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)}-K_0) = 1 + \frac{1}{2V_\infty^{1/2}}\int_{\mathbb{R}} dx\, e^{\pm V_\infty^{1/2}x}[V(x)-V_\infty]\Psi_\pm(0,x) = 0. \tag{3.120}$$

Thus, (3.110) and (3.111) together with (3.118)–(3.120) yield

$$\begin{aligned}\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)}-P_0-K_0) &= -C_0\int_{\mathbb{R}} dx\,[V(x)-V_\infty]\Psi_0(x)\Psi_\pm(0,x) \\ &\quad\times \frac{1}{2V_\infty^{1/2}}\int_{\mathbb{R}} dx\, e^{\pm V_\infty^{1/2}x}[V(x)-V_\infty]\hat\psi_\pm(x)\end{aligned} \tag{3.121}$$

(where the equations for the + and − sign should be read separately). Applying (3.39) for $\lambda_j = 0$ and (3.97) one obtains

$$\begin{aligned}\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0) &= \frac{-1}{2V_\infty^{1/2} C_\pm} \int_{\mathbb{R}} dx\, e^{\pm V_\infty^{1/2} x} [V(x) - V_\infty] \hat{\psi}_\pm(x) \\ &= \frac{-1}{2V_\infty^{1/2}} \int_{\mathbb{R}} dx\, e^{\pm V_\infty^{1/2} x} [V(x) - V_\infty] \psi_\pm(x),\end{aligned} \tag{3.122}$$

using (3.117) in the last line.

To remove the temporary compact support assumption (3.107) we first note that by a standard iteration argument, the Volterra equations

$$\begin{aligned} e^{\pm V_\infty^{1/2} x} \psi_\pm(x) = -e^{\pm V_\infty^{1/2} x} \Psi_\pm(0,x) \mp \frac{1}{2V_\infty^{1/2}} \int_x^{\pm\infty} dx' \left[ e^{\pm 2V_\infty^{1/2}(x-x')} - 1 \right] \\ \times [V(x') - V_\infty] e^{\pm V_\infty^{1/2} x'} \psi_\pm(x'), \quad x \in \mathbb{R}, \end{aligned} \tag{3.123}$$

have unique and bounded solutions on $\mathbb{R}$, which together with their first derivatives are locally absolutely continuous on $\mathbb{R}$, as long as the condition (3.16) is satisfied. This follows since there exists a constant $C > 0$ such that $\left| e^{\pm V_\infty^{1/2} x} \Psi_\pm(0,x) \right| \leq C$, $x \in \mathbb{R}$. Thus, the right-hand side of (3.99) remains well-defined under condition (3.16) on $V$.

Next, similarly to the proof of Theorem 3.6, we choose compactly supported sequences $u_n, v_n \in L^2(\mathbb{R}; dx)$, $n \in \mathbb{N}$, such that $W_n = V_n - V_\infty = u_n v_n$ converges to $W = V - V_\infty = uv$ in $L^1(\mathbb{R}; dx)$ as $n \to \infty$ and introduce the maximally defined operator $H_n$ in $L^2(\mathbb{R}; dx)$ associated with the differential expression $L_n = -(d^2/dx^2) + V_n(x)$, $x \in \mathbb{R}$. Since $H_n$ converges to $H$ in norm resolvent sense (this follows in exactly the same manner as discussed in the proof of Theorem 3.6), the spectrum of $H_n$ converges to that of $H$ as $n \to \infty$. In particular, for $n \in \mathbb{N}$ sufficiently large, $H_n$ has a simple eigenvalue $\lambda_n$ in a small neighborhood of $z = 0$ such that $\lambda_n \underset{n\to\infty}{\longrightarrow} 0$ . Multiplying $V_n$ by a suitable coupling constant $g_n \in \mathbb{R}$, where $g_n \underset{n\to\infty}{\longrightarrow} 1$, then guarantees that the maximally defined operator $H_n(g_n)$ in $L^2(\mathbb{R}; dx)$ associated with the differential expression $L_n(g_n) = -(d^2/dx^2) + g_n V_n(x)$, $x \in \mathbb{R}$, has a simple eigenvalue at $z = 0$, in particular, $0 \in \sigma_{\rm d}(H_n(g_n))$. (Multiplying $V$ by $g_n$ changes the essential spectrum of $H_n(g_n)$ into $[g_n V_\infty, \infty)$, but since $\lambda_n \to 0$ and $g_n \to 1$ as $n \to \infty$, this shift in the essential spectrum is irrelevant in this proof as long as $n \in \mathbb{N}$ is sufficiently large.)

Finally, the approximation arguments described in the proof of Theorem 4.3 of [13] permit one to pass to the limit $n \to \infty$ establishing (3.99) without the extra hypothesis (3.107). □

It remains to show that the two results (3.95) and (3.99) for the Fredholm determinant $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0)$ coincide. This will be undertaken next.

**Theorem 3.9.** *Assume Hypothesis* 3.2 *and suppose* $0 \in \sigma_{\rm d}(H)$. *Then the expressions* (3.95) *and* (3.99) *for* $\det_{L^2(\mathbb{R};dx)}(I_{L^2(\mathbb{R};dx)} - P_0 - K_0)$ *coincide.*

*Proof.* To keep the arguments as short as possible, we first prove that (3.95) and (3.99) coincide under the simplifying compact support assumption (3.107) on $V - V_\infty$. Again, the general case where $V$ satisfies Hypothesis 3.2 then follows from an approximation argument.

More precisely, we suppose that

$$\operatorname{supp}(V - V_\infty) \subset [-R, R] \text{ for some } R > 0. \tag{3.124}$$

Proving that (3.95) and (3.99) coincide is then equivalent to showing that

$$-\int_{-R}^{R} dx\, [V(x) - V_\infty] e^{\pm V_\infty^{1/2} x} \psi_\pm(x) = \int_{-R}^{R} dx\, [V(x) - V_\infty] \Psi_+(0,x) \Psi_-(0,x). \tag{3.125}$$

We start with the right-hand side of (3.125): First we note that

$$\frac{d}{dx} \mathrm{Wr}(\psi_\pm, \Psi_\mp(0))(x) = [V(x) - V_\infty] \Psi_+(0,x) \Psi_-(0,x) \text{ for a.e. } x \in \mathbb{R}, \tag{3.126}$$

where we used that

$$-\psi_\pm''(x) + V(x)\psi_\pm(x) = [V(x) - V_\infty] \Psi_\pm(0,x) \text{ for a.e. } x \in \mathbb{R}, \tag{3.127}$$

which in turn follows by twice differentiating (3.100), and

$$-\Psi_\pm''(0,x) + V(x)\Psi_\pm(0,x) = 0 \text{ for a.e. } x \in \mathbb{R}. \tag{3.128}$$

Thus, one concludes that

$$\begin{aligned}
&\int_{-R}^{R} dx\, [V(x) - V_\infty] \Psi_+(0,x) \Psi_-(0,x) \\
&\quad = \int_{-R}^{R} dx\, \frac{d}{dx} \mathrm{Wr}(\psi_+, \Psi_-(0))(x) \\
&\quad = \mathrm{Wr}(\psi_+, \Psi_-(0))(R) - \mathrm{Wr}(\psi_+, \Psi_-(0))(-R) \\
&\quad = -\mathrm{Wr}(\Psi_+(0), \Psi_-(0))(R) - \mathrm{Wr}(\psi_+, \Psi_-(0))(-R) \\
&\quad = -\mathrm{Wr}(\psi_+, \Psi_-(0))(-R).
\end{aligned} \tag{3.129}$$

Here we employed that

$$\psi_+(x) = -\Psi_+(0,x) \text{ for } x \geq R \tag{3.130}$$

(cf. (3.100)) and

$$2V_\infty^{1/2} \mathcal{F}(0) = \mathrm{Wr}(\Psi_+(0), \Psi_-(0)) = 0 \tag{3.131}$$

since by hypothesis, $0 \in \sigma_{\mathrm{d}}(H)$. Similarly, one computes

$$\begin{aligned}
&\int_{-R}^{R} dx\, [V(x) - V_\infty] \Psi_+(0,x) \Psi_-(0,x) \\
&\quad = \int_{-R}^{R} dx\, \frac{d}{dx} \mathrm{Wr}(\psi_-, \Psi_+(0))(x) \\
&\quad = \mathrm{Wr}(\psi_-, \Psi_+(0))(R) - \mathrm{Wr}(\psi_-, \Psi_+(0))(-R) \\
&\quad = \mathrm{Wr}(\psi_-, \Psi_+(0))(R) + \mathrm{Wr}(\Psi_-(0), \Psi_+(0))(-R) \\
&\quad = \mathrm{Wr}(\psi_-, \Psi_+(0))(R),
\end{aligned} \tag{3.132}$$

where we used

$$\psi_-(x) = -\Psi_-(0,x) \text{ for } x \leq -R \tag{3.133}$$

(cf. (3.100)) and again (3.131). In particular, one concludes that

$$\mathrm{Wr}(\psi_-, \Psi_+(0))(R) = -\mathrm{Wr}(\psi_+, \Psi_-(0))(-R). \tag{3.134}$$

To compute the left-hand side of (3.125) we first note that

$$\begin{aligned}
&\frac{d}{dx}\mathrm{Wr}\Big(\psi_\pm(x), e^{\pm V_\infty^{1/2}x}\Big) + \frac{d}{dx}\mathrm{Wr}\Big(\Psi_\pm(0,x), e^{\pm V_\infty^{1/2}x}\Big) \\
&\quad = -[V(x) - V_\infty]e^{\pm V_\infty^{1/2}x}\psi_\pm(x) \ \text{ for a.e. } x \in \mathbb{R},
\end{aligned} \tag{3.135}$$

where we employed again (3.127) and (3.128). Thus, one infers that

$$\begin{aligned}
&-\int_{-R}^{R} dx\, [V(x) - V_\infty]e^{V_\infty^{1/2}x}\psi_+(x) \\
&\quad = \int_{-R}^{R} dx \left[\frac{d}{dx}\mathrm{Wr}\Big(\psi_+(x), e^{V_\infty^{1/2}x}\Big) + \frac{d}{dx}\mathrm{Wr}\Big(\Psi_+(0,x), e^{V_\infty^{1/2}x}\Big)\right] \\
&\quad = \mathrm{Wr}\Big(\psi_+(x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=R} - \mathrm{Wr}\Big(\psi_+(x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=-R} \\
&\qquad + \mathrm{Wr}\Big(\Psi_+(0,x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=R} - \mathrm{Wr}\Big(\Psi_+(0,x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=-R} \\
&\quad = -\mathrm{Wr}\Big(\Psi_+(0,x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=R} + \mathrm{Wr}\Big(\Psi_+(0,x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=R} \\
&\qquad - \mathrm{Wr}\Big(\psi_+(x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=-R} - \mathrm{Wr}\Big(\Psi_+(0,x), e^{V_\infty^{1/2}x}\Big)\Big|_{x=-R} \\
&\quad = -\mathrm{Wr}(\psi_+, \Psi_-(0))(-R) - \mathrm{Wr}(\Psi_+(0), \Psi_-(0))(-R) \\
&\quad = -\mathrm{Wr}(\psi_+, \Psi_-(0))(-R).
\end{aligned} \tag{3.136}$$

Here we used again (3.130) and (3.131) as well as

$$e^{V_\infty^{1/2}x} = \Psi_-(0,x) \ \text{ for } x \le -R \tag{3.137}$$

(cf. (3.116)). Similarly one computes

$$-\int_{-R}^{R} dx\, [V(x) - V_\infty]e^{-V_\infty^{1/2}x}\psi_-(x) = \mathrm{Wr}(\psi_-, \Psi_+(0))(R). \tag{3.138}$$

Taking into account (3.134), this completes the proof of (3.125). □

3.3. **A formula of Simon.** Finally, we turn to an interesting formula for the Jost solutions $\Psi_\pm(z,\,\cdot\,)$ in terms of Fredholm determinants derived by Simon [37].

To set the stage, we abbreviate $\mathbb{R}_\pm = (0, \pm\infty)$ and introduce the one-dimensional Dirichlet and Neumann Laplacians perturbed by the constant potential $V_\infty$, $H_\pm^{(0),D}$ and $H_\pm^{(0),N}$ in $L^2(\mathbb{R}_\pm; dx)$ by

$$H_\pm^{(0),D} = -\frac{d^2}{dx^2} + V_\infty, \quad \mathrm{dom}\big(H_\pm^{(0),D}\big) = H_0^2(\mathbb{R}_\pm), \tag{3.139}$$

$$H_\pm^{(0),N} = -\frac{d^2}{dx^2} + V_\infty, \quad \mathrm{dom}\big(H_\pm^{(0),N}\big) = \{g \in H^2(\mathbb{R}_\pm) \,|\, g'(0_\pm) = 0\}. \tag{3.140}$$

Next, we recall that

$$\Psi_\pm(z,0) = \det_{L^2(\mathbb{R}_\pm;dx)}\Big(I + u(H_\pm^{(0),D} - z)^{-1}v\Big), \quad \mathrm{Im}\big((z - V_\infty)^{1/2}\big) > 0, \tag{3.141}$$

a celebrated formula by Jost and Pais [20] (in the case $V_\infty = 0$). For more details and background on (3.141) we refer to [13] and the references cited therein.

Moreover, it is known (cf. [12], [13]) that

$$\begin{aligned}\Psi'_\pm(z,0) = \pm i(z-V_\infty)^{1/2}\det{}_{L^2(\mathbb{R}_\pm;dx)}\Big(I + u(H_\pm^{(0),N}-z)^{-1}v\Big),\\ \operatorname{Im}\big((z-V_\infty)^{1/2}\big)>0.\end{aligned} \tag{3.142}$$

We conclude this section by presenting a quick proof of the representation of the Jost solutions $\Psi_\pm(z,x)$ and their $x$-derivatives, $\Psi'_\pm(z,x)$, in terms of symmetrized perturbation determinants, starting from the Jost and Pais formula (3.141) and its analog (3.142) for $\Psi'_\pm(z,0)$:

**Lemma 3.10** ([37]). *Suppose $V$ satisfies* (3.16) *and let* $\operatorname{Im}\big((z-V_\infty)^{1/2}\big)>0$, $x\in\mathbb{R}$. *Then,*

$$\begin{aligned}\Psi_\pm(z,x) &= e^{\pm i(z-V_\infty)^{1/2}x}\\ &\quad\times \det{}_{L^2(\mathbb{R}_\pm;dx)}\Big(I_{L^2(\mathbb{R}_\pm;dx))} + u(\,\cdot\,+x)(H_\pm^{(0),D}-z)^{-1}v(\,\cdot\,+x)\Big),\end{aligned} \tag{3.143}$$

$$\begin{aligned}\Psi'_\pm(z,x) &= \pm i(z-V_\infty)^{1/2}e^{\pm i(z-V_\infty)^{1/2}x}\\ &\quad\times \det{}_{L^2(\mathbb{R}_\pm;dx)}\Big(I_{L^2(\mathbb{R}_\pm;dx))} + u(\,\cdot\,+x)(H_\pm^{(0),N}-z)^{-1}v(\,\cdot\,+x)\Big).\end{aligned} \tag{3.144}$$

*Proof.* Denoting $V_y(x)=V(x+y)$, $x,y\in\mathbb{R}$, and by $\Psi_{y,\pm}(z,\,\cdot\,)$ the Jost solutions associated with $V_y$, an elementary change of variables in the Volterra integral equation (3.43) for $\Psi_{y,\pm}$ yields

$$\begin{aligned}\Psi_{y,\pm}(z,x) &= e^{\mp i(z-V_\infty)^{1/2}y}\Psi_\pm(z,x+y),\\ \Psi'_{y,+}(z,x) &= e^{\mp i(z-V_\infty)^{1/2}y}\Psi'_+(z,x+y).\end{aligned} \tag{3.145}$$

Taking $x=0$ in (3.145) implies

$$\Psi_{y,\pm}(z,0) = e^{\mp i(z-V_\infty)^{1/2}y}\Psi_\pm(z,y), \tag{3.146}$$

$$\Psi'_{y,\pm}(z,0) = e^{\mp i(z-V_\infty)^{1/2}y}\Psi'_\pm(z,y). \tag{3.147}$$

Using the Jost–Pais-type formulas

$$\Psi_{y,\pm}(z,0) = \det{}_{L^2(\mathbb{R}_\pm;dx)}\Big(I + u(\,\cdot\,+y)(H_\pm^{(0),D}-z)^{-1}v(\,\cdot\,+y)\Big), \tag{3.148}$$

$$\Psi'_{y,\pm}(z,0) = \pm i(z-V_\infty)^{1/2}\det{}_{L^2(\mathbb{R}_\pm;dx)}\Big(I + u(\,\cdot\,+y)(H_\pm^{(0),N}-z)^{-1}v(\,\cdot\,+y)\Big), \tag{3.149}$$

an insertion of (3.148) into the left-hand side of (3.146) proves (3.143). Similarly, an insertion of (3.149) into the left-hand side of (3.147) yields (3.144). ☐

## 4. The multi-dimensional case

In the previous section, we have illustrated within the simple setting of one-dimensional scalar reaction–diffusion equations how the stability index may be equally well calculated from an Jost/Evans function point of view, or else, using semi-separability of the integral kernels of Birman–Schwinger-type operators, directly from first principles using Fredholm determinants. We conclude by describing, again within the reaction–diffusion setting, an algorithm for multi-dimensional computations via Fredholm determinants, based on semi-separability of the integral kernels combined with Galerkin approximations.

4.1. **Flow in an infinite cylinder.** Consider a scalar reaction-diffusion equation

$$w_t = \Delta w + f(w), \tag{4.1}$$

on an infinite cylinder $x = (x_1, x_2, \dots, x_d) \in \mathbb{R} \times \Omega$, where $\Delta = \Delta_x$ is the Laplacian in the $x$-variables, $\Omega \subset \mathbb{R}^{d-1}$ is a bounded domain, $w$ and $f$ are real-valued functions,

$$f \in C^3(\mathbb{R}). \tag{4.2}$$

In what follows we will assume that $\Omega = [0, 2\pi]^{d-1}$ and consider only the physical cases $d = 2, 3$. Unless explicitly stated otherwise, we will always assume that periodic boundary conditions are used on the boundary $\partial\Omega$ of $\Omega$ (viewing $\Omega$ as a $(d-1)$-dimensional torus in the following) if $d = 2, 3$. For $x \in \mathbb{R} \times \Omega$ we will always write $x = (x_1, y)$, where $x_1 \in \mathbb{R}$ and $y = (x_2, \dots, x_d) \in \Omega$, and similarly, $x' = (x_1', \dots, x_d') = (x_1', y')$, $y' = (x_2', \dots, x_d')$. We will abbreviate $dx = dx_1 dx_2 \dots dx_d$ and $dy = dx_2 \dots dx_d$, and frequently use the fact that the space $L^2(\mathbb{R} \times \Omega; dx) = L^2\big(\mathbb{R}; dx_1; L^2(\Omega; dy)\big) = L^2\big(\Omega; dy; L^2(\mathbb{R}; dx_1)\big)$ is isometrically isomorphic to the space $\ell^2\big(\mathbb{Z}^{d-1}; L^2(\mathbb{R}; dx_1)\big)$ via the discrete Fourier transform in the $y$-variables:

$$w(x) = \sum_{j \in \mathbb{Z}^{d-1}} \hat{w}_j(x_1) e^{ij \cdot y}, \quad x = (x_1, y) \in \mathbb{R} \times \Omega, \tag{4.3}$$

where

$$\hat{w}_j(x_1) = (2\pi)^{1-d} \int_\Omega dy\, w(x_1, y) e^{-ij \cdot y}, \quad x_1 \in \mathbb{R}. \tag{4.4}$$

4.1.1. *Galerkin-based Evans function.* We first review the Galerkin approach described in [23], in which a standard Evans function is defined for a one-dimensional truncation of the linearized operator about a standing-wave solution in a series of remarks.

**Remark 4.1.** Under our standing assumption of periodic boundary conditions on $\partial\Omega$, there exist planar steady-state solutions $U = U(x_1)$, where $U$ is the solution of the corresponding one-dimensional problem (3.4) described in Section 3. Linearizing about $U$, cf. (3.1)–(3.9), denoting $V(x_1) = -f'(U(x_1))$, and taking the discrete Fourier transform in directions $x_2, \dots, x_d$, one obtains a decoupled family of one-dimensional eigenvalue problems

$$0 = (L_j - \lambda)\psi = \left(\frac{d^2}{dx_1^2} - |j|^2 - \lambda - V(x_1)\right)\psi, \tag{4.5}$$

indexed by Fourier frequencies $j = (j_2, \dots, j_d) \in \mathbb{Z}^{d-1}$, each of which possess a well-defined Evans function and stability index. At $j = 0$ and $\lambda = 0$, there is an eigenfunction $U'(x_1)$ associated with translation invariance in the $x_1$-direction of the underlying equations; for other $j$, there is typically no eigenfunction at $\lambda = 0$. Asymptotic analysis as in [1], [30] yields a trivial, positive stability index for $|j|$ sufficiently large, so that computations may be truncated at a finite value of $|j|$.

**Remark 4.2.** In the above example, the operators $L_j$ are real-valued (i.e., map real-valued functions into real-valued ones), hence a stability index makes sense. For more general, non-selfadjoint operators, one may expand in sines and cosines to obtain a family of real-valued eigenvalue equations for which a stability index may again be defined. This principle extends further to generalized Fourier expansions in the case of general $\Omega$, requiring only real-valuedness (in the above sense) of the original (multi-dimensional) operator $L$.

**Remark 4.3.** More generally, consider a standing-wave solution $U = U(x)$ that is not planar, but only converges as $x_1 \to \pm\infty$ to a constant state $U_\infty$. We assume

$$\big(x_1 \mapsto \|U(x_1, \,\cdot\,)\|_{H^{3/2}(\Omega)}\big) \in \big(L^1 \cap L^\infty\big)(\mathbb{R}; dx_1). \tag{4.6}$$

This writing means that the map $x_1 \mapsto U(x_1, \,\cdot\,)$ from $\mathbb{R}$ into the fractional Sobolev space $H^{3/2}(\Omega)$ is both an $L^1$- and $L^\infty$-function with respect to the variable $x_1$. Linearizing about $U$, denoting by $\psi = \psi(x)$ the corresponding eigenfunction, and taking the Fourier transform in directions $x_2, \dots, x_d$, one obtains a coupled family of one-dimensional eigenvalue problems

$$0 = \left(\frac{d^2}{dx_1^2} - |j|^2 - \lambda\right)\hat\psi_j - \big(\widehat{V}(x_1, \,\cdot\,) * \hat\psi_{(\,\cdot\,)}\big)(j), \quad j \in \mathbb{Z}^{d-1}. \tag{4.7}$$

Here $*$ denotes convolution in $j$,

$$\psi(x) = \sum_{j \in \mathbb{Z}^{d-1}} \hat\psi_j(x_1) e^{ij\cdot y}, \quad x = (x_1, y) \in \mathbb{R} \times \Omega, \tag{4.8}$$

and $\widehat{V}(x_1, j)$ denotes the value of the Fourier transform of $V(x_1, \,\cdot\,)$ in the variable $y = (x_2, \dots, x_d)$. Following the approach of [23], one may proceed by *Galerkin approximation*, truncating the system at some sufficiently high-order mode $|j| \leqslant J$, to obtain again a very large, but finite, real-valued eigenvalue ODE in $x_1$, for which one may define in the usual way an Evans function and a stability index.

**Remark 4.4.** While we focus primarily on periodic boundary conditions on $\partial\Omega$ throughout this section, one can treat other boundary conditions such as Dirichlet, Neumann, or more generally, Robin-type boundary conditions in an analogous fashion. The key fact used in (4.3) and (4.4) is the eigenfunction expansion associated with the discrete eigenvalue problem of the self-adjoint Laplacian in $L^2(\Omega; dy))$ with periodic boundary conditions on $\partial\Omega$. The latter can be replaced by analogous discrete eigenvalue problems of the Laplacian with other self-adjoint boundary conditions on $\partial\Omega$.

4.1.2. *Fredholm determinant version.* We now describe an alternative method based on the Fredholm determinant, in which the Jost and Evans functions are prescribed canonically as characteristic determinants, but computed by Galerkin approximation: that is, we approximate the determinant rather than the system of equations.

Specifically, consider again the general situation of Remark 4.3 of a solution $U$ of (4.1) decaying as $x_1 \to \pm\infty$ to some constant state $U_\infty$. As in (3.9), we denote $V(x) = -f'(U(x))$, $x \in \Omega \times \mathbb{R}$, and assume that

$$V_\infty = -f'(U_\infty) > 0. \tag{4.9}$$

We define the Birman–Schwinger operator $K(z)$ similarly to (3.26), (3.22) as

$$K(z) = -u(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega; dx)})^{-1} v, \quad z \in \mathbb{C}\backslash[V_\infty, \infty), \tag{4.10}$$

with $H^{(0)}_{\Omega,\mathrm{p}}$ the self-adjoint realization of the differential expression $-\Delta_x + V_\infty$ in $L^2(\mathbb{R} \times \Omega; dx)$ with periodic boundary conditions on $\partial\Omega$, and

$$u(x) = \operatorname{sgn}(V(x) - V_\infty) v(x), \quad v(x) = |V(x) - V_\infty|^{1/2} \tag{4.11}$$

for a.e. $x \in \mathbb{R}\times\Omega$.

For later reference, we define also the asymmetric rearrangement of $K(z)$ by the formula

$$\begin{aligned}\mathcal{K}(z) &= -\big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}uv\\ &= -\big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(V-V_\infty), \quad z\in\mathbb{C}\backslash[V_\infty,\infty).\end{aligned} \tag{4.12}$$

Then, under the assumption

$$\big(x_1 \mapsto \|V(x_1,\,\cdot\,)-V_\infty\|_{L^\infty(\Omega;dy)}\big) \in \big(L^1\cap L^\infty\big)(\mathbb{R};dx_1), \tag{4.13}$$

we have the following result generalizing the one-dimensional case [11, Lemma 2.9]. Fix $z\in\mathbb{C}\backslash[V_\infty,\infty)$. Passing to adjoint operators, if needed, with no loss of generality we will assume below that $\mathrm{Im}(z)\geqslant 0$ and fix the branch of the square root such that $\mathrm{Re}\big((V_\infty+|j|^2-z)^{1/2}\big)>0$ for each $j\in\mathbb{Z}^{d-1}$, a choice consistent with the choice of $Q$ in (4.95).

**Lemma 4.5.** *Assume* (4.13). *If dimensions $d\leqslant 3$ then $K(z), \mathcal{K}(z)\in\mathcal{B}_2\big(L^2(\mathbb{R}\times\Omega;dx)\big)$ for each $z\in\mathbb{C}\backslash[V_\infty,\infty)$. Moreover, the condition on the dimensions is sharp.*

*Proof.* The operator $H^{(0)}_{\Omega,\mathrm{p}}$, since constant-coefficient, decouples under the Fourier transform in the variables $x_2,\dots,x_d$. Consequently, the integral kernel of the resolvent of $H^{(0)}_{\Omega,\mathrm{p}}$, denoted by $\big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(x,x')$, may be found explicitly by a Fourier expansion and, using (3.27), can be expressed as a countable sum of scalar integral kernels:

$$\begin{aligned}&\big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(x,x')\\ &\quad=\frac{i}{2}\sum_{j\in\mathbb{Z}^{d-1}}(z-V_\infty-|j|^2)^{-1/2}e^{i(z-V_\infty-|j|^2)^{1/2}|x_1-x_1'|}e^{ij\,\cdot\,(y-y')},\\ &\qquad\qquad\qquad x=(x_1,y), x'=(x_1',y')\in\mathbb{R}\times\Omega,\end{aligned} \tag{4.14}$$

where $y=(x_2,\dots,x_d)\in\Omega$, $y'=(x_2',\dots,x_d')\in\Omega$, and $j\in\mathbb{Z}^{d-1}$ denote the Fourier wave numbers in these directions. Using Parseval's identity, we obtain for any fixed $x'\in\mathbb{R}\times\Omega$ that

$$\begin{aligned}&\big\|\big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(\,\cdot\,,x')\big\|^2_{L^2(\mathbb{R}\times\Omega;dx)}\\ &\quad=\frac14\sum_{j\in\mathbb{Z}^{d-1}}\int_{\mathbb{R}}dx_1\left|(z-V_\infty-|j|^2)^{-1/2}e^{i(z-V_\infty-|j|^2)^{1/2}|x_1-x_1'|}\right|^2\\ &\quad=\frac14\sum_{j\in\mathbb{Z}^{d-1}}\big|z-V_\infty-|j|^2\big|^{-1}\int_{\mathbb{R}}dx_1\,e^{-2\mathrm{Im}((z-V_\infty-|j|^2)^{1/2})|x_1-x_1'|}\\ &\quad=\frac14\sum_{j\in\mathbb{Z}^{d-1}}\big|z-V_\infty-|j|^2\big|^{-3/2}\Big(\sin\tfrac12\big(\arg(z-V_\infty-|j|^2)\big)\Big)^{-1},\end{aligned} \tag{4.15}$$

where $\mathrm{Im}\big((z-V_\infty-|j|^2)^{1/2}\big)>0$ for $z\in\mathbb{C}\backslash[V_\infty,\infty)$ due to $\mathrm{Im}(z)\geqslant 0$. Since $\arg\big(z-V_\infty-|j|^2\big)\to\pi$ as $|j|\to\infty$, there is a constant $c=c(z)$ such that

$$\big\|\big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(\,\cdot\,,x')\big\|^2_{L^2(\mathbb{R}\times\Omega;dx)}\leqslant c\sum_{j\in\mathbb{Z}^{d-1}}(V_\infty+|j|^2)^{-3/2}, \tag{4.16}$$

hence is finite if and only if $d \leqslant 3$. We recall the formula for the Hilbert–Schmidt norm of the Hilbert–Schmidt operator $K$ with integral kernel $K(x,x')$ (see, e.g., [38, Thm. 2.11], [46, Sect. 1.6.5]):

$$\|K\|_{\mathcal{B}_2(L^2(\mathbb{R}\times\Omega;dx))} = \|K(\,\cdot\,,\,\cdot\,)\|_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dxdx')}. \tag{4.17}$$

Using (4.17) and (4.16) to estimate the integral kernels of (4.10) and (4.12), one infers

$$\begin{aligned}
&\|K(z,\,\cdot\,,\,\cdot\,)\|^2_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dxdx')} \\
&\quad \leqslant \Big\| u(\,\cdot\,) \big\| \big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(\,\cdot\,,\,\cdot\,) \big\|_{L^2(\mathbb{R}\times\Omega;dx')} \Big\|^2_{L^2(\mathbb{R}\times\Omega;dx)} \|v\|^2_{L^\infty(\mathbb{R}\times\Omega;dx')} \\
&\quad \leqslant c \sum_{j\in\mathbb{Z}^{d-1}} (V_\infty + |j|^2)^{-3/2} \;\cdot\; \|u\|^2_{L^2(\mathbb{R}\times\Omega;dx)} \|v\|^2_{L^\infty(\mathbb{R}\times\Omega;dx')},
\end{aligned} \tag{4.18}$$

$$\begin{aligned}
&\|\mathcal{K}(z,\,\cdot\,,\,\cdot\,)\|^2_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dxdx')} \\
&\quad \leqslant \Big\| \big\| \big(H^{(0)}_{\Omega,\mathrm{p}} - zI_{L^2(\mathbb{R}\times\Omega;dx)}\big)^{-1}(\,\cdot\,,\,\cdot\,) \big\|_{L^2(\mathbb{R}\times\Omega;dx)} u(\,\cdot\,)v(\,\cdot\,) \Big\|^2_{L^2(\mathbb{R}\times\Omega;dx')} \\
&\quad \leqslant c \sum_{j\in\mathbb{Z}^{d-1}} (V_\infty + |j|^2)^{-3/2} \;\cdot\; \|uv\|^2_{L^2(\mathbb{R}\times\Omega;dx')},
\end{aligned} \tag{4.19}$$

and finds that $K(z)$ and $\mathcal{K}(z)$ are Hilbert–Schmidt operators for $d \leqslant 3$, as claimed. In the decoupled case, where $u = u(x_1)$, $v = v(x_1)$, these estimates are sharp, showing that in general $K(z)$, $\mathcal{K}(z)$ are Hilbert–Schmidt only for $d \leqslant 3$. ☐

**Definition 4.6.** *Assume* (4.13). *Generalizing the one-dimensional case* (3.50)*, we introduce in dimensions* $d = 2, 3$*, a* 2-modified *Jost function defined by*

$$\mathcal{F}_2(z) = \det{}_{2,L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}(z)), \quad z \in \mathbb{C}\backslash[V_\infty,\infty). \tag{4.20}$$

By the determinant property (2.42) one then obtains

$$\mathcal{F}_2(z) = \det{}_{2,L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - K(z)), \quad z \in \mathbb{C}\backslash[V_\infty,\infty), \tag{4.21}$$

which could equivalently have been used to define $\mathcal{F}_2(z)$.

**Remark 4.7.** Similar to Lemma 4.5 calculations show that $K(z)$ belongs to successively weaker trace ideal classes as $d$ increases, for which a higher-modified Jost function may be defined as a higher-modified Fredholm determinant. We restrict our attention here to the main physical cases $d = 2, 3$.

**Remark 4.8.** Comparing with formula (3.50) for the *non-modified* Jost function given in the one-dimensional $d = 1$ case (when $K(z)$ and $\mathcal{K}(z)$ are trace-class operators), (2.41) implies the relation

$$\begin{aligned}
&\det{}_{2,L^2(\mathbb{R};dx_1)}(I_{L^2(\mathbb{R};dx_1)} - K(z)) \\
&\quad = \det{}_{L^2(\mathbb{R};dx_1)}(I_{L^2(\mathbb{R};dx_1)} - K(z)) e^{\operatorname{tr}_{L^2(\mathbb{R};dx_1)}(K(z))}.
\end{aligned} \tag{4.22}$$

Thus, (4.20) differs from (3.50) by a nonvanishing analytic factor $e^{\operatorname{tr}_{L^2(\mathbb{R};dx_1)}(K(z))}$, and hence for practical purposes the use of $\det_{2,L^2(\mathbb{R};dx_1)}(\,\cdot\,)$ and $\det_{L^2(\mathbb{R};dx_1)}(\,\cdot\,)$ in (4.20) for $d = 1$ are equivalent. For $d > 1$ we make a related comment in Remark 4.14.

4.1.3. *Galerkin approximations.* Next, we approximate $\mathcal{F}_2$ by a Galerkin approximation, working for convenience with the asymmetric version (4.20). We will augment (4.13) with the more restrictive, but still typically satisfied, condition

$$\big(x_1 \mapsto \|V(x_1,\,\cdot\,) - V_\infty\|_{H^{3/2}(\Omega)}\big) \in L^2(\mathbb{R}; dx_1). \tag{4.23}$$

As in (3.17), we introduce

$$W(x) = V(x) - V_\infty, \quad x \in \mathbb{R}\times\Omega, \tag{4.24}$$

and expand $W$ into a Fourier series in variables $y = (x_2, \dots, x_d)$ so that

$$W(x) = \sum_{m\in\mathbb{Z}^{d-1}} \widehat{W}_m(x_1)e^{im\,\cdot\,y}, \quad x = (x_1, y) \in \mathbb{R}\times\Omega. \tag{4.25}$$

Substituting (4.14) into (4.12), we obtain an expansion of the integral kernel of the operator $\mathcal{K}(z)$:

$$\mathcal{K}(z,x,x') = -\sum_{j\in\mathbb{Z}^{d-1}} e^{ij\,\cdot\,y}\,\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\,(V(x')-V_\infty)e^{-ij\,\cdot\,y'} \tag{4.26}$$

$$= -\sum_{j,m\in\mathbb{Z}^{d-1}} e^{ij\,\cdot\,y}\,\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\,\widehat{W}_{j-m}(x_1')e^{-im\,\cdot\,y'}. \tag{4.27}$$

Introducing

$$\begin{aligned} f_1^j(x) &= -2^{-1}e^{ij\,\cdot\,y}(V_\infty+|j|^2-z)^{-1/2}e^{(V_\infty+|j|^2-z)^{1/2}x_1},\\ f_2^j(x) &= -2^{-1}e^{ij\,\cdot\,y}(V_\infty+|j|^2-z)^{-1/2}e^{-(V_\infty+|j|^2-z)^{1/2}x_1},\\ g_1^j(x') &= e^{-(V_\infty+|j|^2-z)^{1/2}x_1'}(V(x_1')-V_\infty)e^{-ij\,\cdot\,y'},\\ g_2^j(x') &= e^{(V_\infty+|j|^2-z)^{1/2}x_1'}(V(x_1')-V_\infty)e^{-ij\,\cdot\,y'}, \end{aligned} \tag{4.28}$$

we obtain from (4.26) an expansion of $\mathcal{K}(z,x,x')$ as a countable sum

$$\mathcal{K}(z,x,x') = \begin{cases} \sum_{j\in\mathbb{Z}^{d-1}} f_1^j(x)g_1^j(x'), & x_1' > x_1,\\ \sum_{j\in\mathbb{Z}^{d-1}} f_2^j(x)g_2^j(x'), & x_1 > x_1', \end{cases} \tag{4.29}$$

of scalar integral kernels that are semi-separable in $x_1$.

Truncating (4.27) at some finite wave number $J$ or, equivalently, Fourier expanding $f_k^j$, $g_k^j$ in (4.29) in variables $y$ and $y'$ and truncating the resulting series at some finite wave number $J$, we obtain a sequence of Galerkin approximations

$$\mathcal{K}_J(z,x,x') = -\sum_{|m|,|j|\leqslant J} e^{ij\,\cdot\,y}\,\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\,\widehat{W}_{j-m}(x_1')e^{-im\,\cdot\,y'} \tag{4.30}$$

$$= \begin{cases} \displaystyle\sum_{|m|,|j|\leqslant J} e^{ij\,\cdot\,y}\big(\widehat{f_1^j}\big)_j(x_1)\big(\widehat{g_1^j}\big)_{-m}(x_1')e^{-im\,\cdot\,y'}, & x_1' > x_1,\\ \displaystyle\sum_{|m|,|j|\leqslant J} e^{ij\,\cdot\,y}\big(\widehat{f_2^j}\big)_j(x_1)\big(\widehat{g_2^j}\big)_{-m}(x_1')e^{-im\,\cdot\,y'}, & x_1 > x_1', \end{cases} \tag{4.31}$$

where $\big(\widehat{f_k^j}\big)_m$ denote the Fourier coefficients of

$$f_k^j(x_1,y) = \sum_{m\in\mathbb{Z}^{d-1}} \big(\widehat{f_k^j}\big)_m e^{im\,\cdot\,y} = \big(\widehat{f_k^j}\big)_j e^{ij\,\cdot\,y}, \tag{4.32}$$

and

$$\big(\widehat{g_k^j}\big)_m(x_1') = \widehat{W}_{j+m}(x_1')e^{(-1)^{k+1}(V_\infty+|j|^2-z)^{1/2}x_1'}, \quad k=1,2, \tag{4.33}$$

denote the Fourier coefficients of the function

$$g_k^j(x') = e^{(-1)^{k+1}(V_\infty+|j|^2-z)^{1/2}x_1'}W(x')e^{-ij\cdot y'}, \quad k=1,2. \tag{4.34}$$

We denote by $\mathcal{K}_J(z)$ the integral operator on $L^2(\mathbb{R}\times\Omega;dx)$ with the integral kernel (4.30), (4.31).

**Theorem 4.9.** *Let $z\in\mathbb{C}\backslash[V_\infty,\infty)$. Then under assumptions* (4.13) *and* (4.23), *$\mathcal{K}_J(z)\in\mathcal{B}_2\big(L^2(\mathbb{R}\times\Omega;dx)\big)$ for dimensions $d=2,3$. Moreover, for $d=2,3$, $\mathcal{K}_J(z)$ converges in the Hilbert–Schmidt norm to $\mathcal{K}(z)$ at rate $J^{(d-4)/4}$ as $J\to\infty$ and hence the sequence $\mathcal{F}_{2,J}(z)$ defined by*

$$\mathcal{F}_{2,J}(z) = {\det}_{2,L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z)), \tag{4.35}$$

*converges to $\mathcal{F}_2(z) = {\det}_{2,L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)}-\mathcal{K}(z))$ as $J\to\infty$ at rate $J^{(d-4)/4}$.*

*Proof.* Using (4.27) and (4.30), one obtains

$$\begin{aligned}\mathcal{K}(z,x,x') - \mathcal{K}_J(z,x,x') &= -\bigg(\sum_{|j|=0}^{J}\sum_{|m|=J+1}^{\infty} + \sum_{|j|=J+1}^{\infty}\sum_{|m|=0}^{\infty}\bigg) \\ &\quad\times\Big(2^{-1}e^{ij\cdot y}(V_\infty+|j|^2-z)^{-1/2}e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}\widehat{W}_{j-m}(x_1')e^{-im\cdot y'}\Big).\end{aligned} \tag{4.36}$$

By the triangle inequality and Parseval's identity one therefore infers

$$\begin{aligned}&\frac{1}{2}\|\mathcal{K}(z)-\mathcal{K}_J(z)\|^2_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dx\times dx')} \\ &\quad\leqslant \bigg\|\sum_{|j|=0}^{J}\sum_{|m|=J+1}^{\infty}(\,\cdot\,)\bigg\|^2_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dxdx')} \\ &\qquad+ \bigg\|\sum_{|j|=J+1}^{\infty}\sum_{|m|=0}^{\infty}(\,\cdot\,)\bigg\|^2_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dxdx')} \\ &\quad= \sum_{|j|=0}^{J}\sum_{|m|=J+1}^{\infty}\bigg\|\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\widehat{W}_{j-m}(x_1')\bigg\|^2_{L^2(\mathbb{R}\times\mathbb{R};dx_1dx_1')} && (4.37)\\ &\qquad+ \sum_{|j|=J+1}^{\infty}\sum_{|m|=0}^{\infty}\bigg\|\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\widehat{W}_{j-m}(x_1')\bigg\|^2_{L^2(\mathbb{R}\times\mathbb{R};dx_1dx_1')}. && (4.38)\end{aligned}$$

We will now estimate (4.37) and (4.38) separately. Using arguments similar to (4.15)–(4.16), one observes that the sum in (4.37) can be estimated as follows:

$$\begin{aligned}(4.37) &= \sum_{|j|=0}^{J}\bigg\|\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|\,\cdot\,|}}{2(V_\infty+|j|^2-z)^{1/2}}\bigg\|^2_{L^2(\mathbb{R};dx_1)}\sum_{|m|=J+1}^{\infty}\big\|\widehat{W}_{j-m}(\,\cdot\,)\big\|^2_{L^2(\mathbb{R};dx_1')} \\ &\leqslant c\sum_{j\in\mathbb{Z}^{d-1}}(V_\infty+|j|^2)^{-3/2}\sum_{|m|=J+1}^{\infty}\big\|\widehat{W}_m(\,\cdot\,)\big\|^2_{L^2(\mathbb{R};dx_1')} \\ &= c'\|W-W_J\|^2_{L^2(\mathbb{R}\times\Omega;dx')}.\end{aligned} \tag{4.39}$$

In the last equality we used that the series $\sum_{j\in\mathbb{Z}^{d-1}} |j|^{-3}$ converges due to $1 \leqslant d \leqslant 3$, and Parseval's identity for $W - W_J$, where

$$W_J(x) = \sum_{|m|\leqslant J} \widehat{W}_m(x_1)e^{im\cdot y}, \quad x = (x_1, y) \in \mathbb{R}\times\Omega, \tag{4.40}$$

is the truncation of $W$. By the Sobolev embedding $W^{3/2,2}(\Omega) \hookrightarrow W^{3/4,4}(\Omega)$ (cf., e.g., [19, Theorem 1.6.1], [42, p. 328, Eq. (8)], [44, Sects. I.4–I.6]) and a standard Cauchy–Schwartz argument, one infers for each $x_1 \in \mathbb{R}$,

$$\begin{aligned}
&\|W(x_1,\cdot\,) - W_J(x_1,\cdot\,)\|^2_{L^2(\Omega;dy)} = \sum_{|j|>J} \big|\widehat{W}_j(x_1)\big|^2 = \sum_{|j|>J} |j|^{3/2}\big|\widehat{W}_j(x_1)\big|^2|j|^{-3/2}\\
&\leqslant \bigg(\sum_{|j|>J} |j|^3\big|\widehat{W}_j(x_1)\big|^4\bigg)^{1/2}\bigg(\sum_{|j|>J}|j|^{-3}\bigg)^{1/2}\\
&\leqslant \|W(x_1,\cdot\,)\|^2_{W^{3/4,4}(\Omega)}\bigg(\sum_{|j|>J}|j|^{-3}\bigg)^{1/2}\\
&\leqslant c\|W(x_1,\cdot\,)\|^2_{H^{3/2}(\Omega)}J^{(d-4)/2},
\end{aligned} \tag{4.41}$$

Here we used standard notation $W^{s,2}(\,\cdot\,) = H^s(\,\cdot\,)$ for Sobolev spaces. Thus, by (4.39),

$$(4.37) \ \leqslant C_1\|W\|^2_{L^2\left(\mathbb{R};dx_1;H^{3/2}(\Omega)\right)}J^{(d-4)/2}. \tag{4.42}$$

Likewise, similarly to (4.15)–(4.16), one observes that the sum in (4.38) can be estimated as follows:

$$\begin{aligned}
(4.38) = &\sum_{|j|=J+1}^{\infty}\bigg\|\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|\cdot|}}{2(V_\infty+|j|^2-z)^{1/2}}\bigg\|^2_{L^2(\mathbb{R};dx_1)}\sum_{|m|=0}^{\infty}\big\|\widehat{W}_{j-m}(\,\cdot\,)\big\|^2_{L^2(\mathbb{R};dx_1')}\\
&\leqslant c\sum_{|j|=J+1}^{\infty}(V_\infty+|j|^2)^{-3/2}\sum_{|m|=0}^{\infty}\big\|\widehat{W}_m(\,\cdot\,)\big\|^2_{L^2(\mathbb{R};dx_1')}\\
&\leqslant c'\sum_{|j|=J+1}^{\infty}|j|^{-3}\,\|W\|^2_{L^2(\mathbb{R}\times\Omega;dx')} \leqslant C_2J^{d-4}\|W\|^2_{L^2(\mathbb{R}\times\Omega;dx')}.
\end{aligned} \tag{4.43}$$

Combining (4.37), (4.38), (4.42), (4.43), and using [46, Section 1.6.5] as in (4.17), one arrives at the estimate

$$\|\mathcal{K}-\mathcal{K}_J\|^2_{L^2((\mathbb{R}\times\Omega)\times(\mathbb{R}\times\Omega);dxdx')} \leqslant 2\|W\|^2_{L^2(\mathbb{R}\times\Omega;dx')}\big(C_1J^{(d-4)/2}+C_2J^{d-4}\big), \tag{4.44}$$

yielding the claimed result. □

Next, we take a closer look at properties of the integral operator $\mathcal{K}_J(z)$ in $L^2(\mathbb{R}\times\Omega;dx)$ with integral kernel given by (4.30), assuming at first that

$$\widehat{W}_{j-m} \in L^2(\mathbb{R};dx_1), \quad m,j\in\mathbb{Z},\ |m|,|j|\leqslant J. \tag{4.45}$$

Using the fact that $L^2(\mathbb{R}\times\Omega;dx)$ decomposes into

$$L^2(\mathbb{R}\times\Omega;dx) = L^2(\mathbb{R};dx_1)\otimes L^2(\Omega;dy), \tag{4.46}$$

we will exploit the natural tensor product structure of the individual terms $\mathcal{K}_{m,j}(z)$ in

$$\mathcal{K}_J(z) = \sum_{|m|,|j|\leqslant J} \mathcal{K}_{m,j}(z), \quad z\in\mathbb{C}\backslash[V_\infty,\infty), \tag{4.47}$$

where $\mathcal{K}_{m,j}(z)$, $m,j\in\mathbb{Z}^{d-1}$, $|m|,|j|\leqslant J$, are integral operators in $L^2(\mathbb{R}\times\Omega;dx)$ with integral kernels given by

$$\begin{split}\mathcal{K}_{m,j}(z,x,x') = -e^{ij\cdot y}\,\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\,\widehat{W}_{j-m}(x_1')e^{-im\cdot y'},\\ z\in\mathbb{C}\backslash[V_\infty,\infty),\ m,j\in\mathbb{Z}^{d-1},\ |m|,|j|\leqslant J.\end{split} \tag{4.48}$$

With respect to the tensor product structure (4.46), the operators $\mathcal{K}_{m,j}(z)$ decompose as

$$\mathcal{K}_{m,j}(z) = \mathcal{A}_{m,j}(z)\otimes\mathcal{B}_{m,j}, \quad z\in\mathbb{C}\backslash[V_\infty,\infty), \tag{4.49}$$

where the operator

$$\mathcal{A}_{m,j}(z) = \overline{\big(-(d^2/dx_1^2)+(V_\infty+|j|^2-z)I_{L^2(\mathbb{R};dx_1)}\big)^{-1}\widehat{W}_{j-m}}, \quad z\in\mathbb{C}\backslash[V_\infty,\infty), \tag{4.50}$$

in $L^2(\mathbb{R};dx_1)$ has the integral kernel

$$\mathcal{A}_{m,j}(z,x_1,x_1') = -\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}}\,\widehat{W}_{j-m}(x_1'), \tag{4.51}$$

and $\mathcal{B}_{m,j}$ in $L^2(\Omega;dy)$ has the integral kernel

$$\mathcal{B}_{m,j}(y,y') = e^{ij\cdot y}\,e^{-im\cdot y'}. \tag{4.52}$$

In particular, each $\mathcal{B}_{m,j}$ is a rank-one and hence trace class operator on $L^2(\Omega;dy)$,

$$\mathcal{B}_{m,j}\in\mathcal{B}_1\big(L^2(\Omega;dy)\big). \tag{4.53}$$

Next, $\mathcal{A}_{m,j}(z)$ is a Hilbert–Schmidt operator on $L^2(\mathbb{R};dx_1)$,

$$\mathcal{A}_{m,j}(z)\in\mathcal{B}_2\big(L^2(\mathbb{R};dx_1)\big), \quad z\in\mathbb{C}\backslash[V_\infty,\infty), \tag{4.54}$$

if and only if (cf., [38, Thm. 2.11], [46, Sect. 1.6.5] and (4.17))

$$\widehat{W}_{j-m}\in L^2(\mathbb{R};dx_1). \tag{4.55}$$

In addition, applying [38, Theorem 4.5, Lemma 4.7], $\mathcal{A}_{m,j}(z)$ is a trace class operator on $L^2(\mathbb{R};dx_1)$,

$$\mathcal{A}_{m,j}(z)\in\mathcal{B}_1\big(L^2(\mathbb{R};dx_1)\big), \quad z\in\mathbb{C}\backslash[V_\infty,\infty), \tag{4.56}$$

if and only if

$$\widehat{W}_{j-m}\in\ell^1\big(L^2(\mathbb{R};dx_1)\big). \tag{4.57}$$

Here the Birman–Solomyak space $\ell^1\big(L^2(\mathbb{R};dx_1)\big)$ is defined by

$$\ell^1\big(L^2(\mathbb{R};dx_1)\big) = \bigg\{f\in L^2_{\rm loc}(\mathbb{R})\,\bigg|\,\sum_{n\in\mathbb{Z}}\bigg(\int_{Q_n}dx_1\,|f(x_1)|^2\bigg)^{1/2}<\infty\bigg\}, \tag{4.58}$$

with $Q_n$ the unit cube in $\mathbb{R}$ centered at $n\in\mathbb{Z}$. We recall that (cf. [38, Ch. 4])

$$\begin{split}&L^1(\mathbb{R};(1+|x_1|)^\delta dx_1)\subsetneqq\ell^1\big(L^2(\mathbb{R};dx_1)\big)\subsetneqq L^1(\mathbb{R};dx_1)\cap L^2(\mathbb{R};dx_1)\\ &\text{for all } \delta>1/2.\end{split} \tag{4.59}$$

We note in passing, that the symmetrized version $A_{m,j}(z)$ of $\mathcal{A}_{m,j}(z)$, given by

$$A_{m,j}(z) = \overline{\hat{u}_{j-m}\big( -(d^2/dx_1^2) + (V_\infty + |j|^2 - z)I_{L^2(\mathbb{R};dx_1)}\big)^{-1}\hat{v}_{j-m}}, \quad z \in \mathbb{C}\backslash[V_\infty, \infty), \tag{4.60}$$

where

$$\hat{u}_{j-m}(x_1) = \operatorname{sgn}\big(\widehat{W}_{j-m}(x_1)\big)\hat{v}_{j-m}(x_1), \quad \hat{v}_{j-m}(x_1) = \big|\widehat{W}_{j-m}(x_1)\big|^{1/2} \tag{4.61}$$

for a.e. $x_1 \in \mathbb{R}$, is a trace class operator under the weaker assumption

$$\widehat{W}_{j-m} \in L^1(\mathbb{R}; dx_1). \tag{4.62}$$

Given these preparations, we can now summarize Hilbert–Schmidt and trace class properties of $\mathcal{K}_J(z)$ as follows:

**Lemma 4.10.** *Assume $z \in \mathbb{C}\backslash[V_\infty, \infty)$. Then,*
*(i) $\mathcal{K}_J(z)$ is a Hilbert–Schmidt operator on $L^2(\mathbb{R}\times\Omega; dx)$ if $\widehat{W}_{j-m} \in L^2(\mathbb{R}; dx_1)$ for all $m, j \in \mathbb{Z}$, $|m|, |j| \leqslant J$.*
*(ii) $\mathcal{K}_J(z)$ is a trace class operator on $L^2(\mathbb{R}\times\Omega; dx)$ if $\widehat{W}_{j-m} \in \ell^1\big(L^2(\mathbb{R}; dx_1)\big)$ for all $m, j \in \mathbb{Z}$, $|m|, |j| \leqslant J$.*

*Proof.* Since the sum in (4.47) is finite, it suffices to prove the Hilbert–Schmidt and trace class properties of $\mathcal{K}_{m,j}(z)$ for fixed $m, j$. Since by (4.49),

$$|\mathcal{K}_{m,j}(z)| = |\mathcal{A}_{m,j}(z)| \otimes |\mathcal{B}_{m,j}|, \tag{4.63}$$

where as usual, $|T| = (T^*T)^{1/2}$, the singular values of $\mathcal{K}_{m,j}(z)$ (i.e., the eigenvalues of $|\mathcal{K}_{m,j}(z)|$) are square summable, respectively, summable, if and only if the singular values of $\mathcal{A}_{m,j}(z)$ are square summable, respectively, summable, since $\mathcal{B}_{m,j}$ is a rank-one operator and hence has precisely one nonzero singular value. This follows from the well-known fact that the spectrum of a tensor product $A_1 \otimes A_2$ in $\mathcal{H}_1 \otimes \mathcal{H}_2$ of bounded operators $A_j$ in the complex separable Hilbert spaces $\mathcal{H}_j$, $j = 1, 2$, is given by the product of the individual spectra (cf., e.g., [32, Theorem XIII.34]), that is,

$$\begin{aligned} \sigma(A_1 \otimes A_2) &= \sigma(A_1) \cdot \sigma(A_2) \\ &= \{\lambda \in \mathbb{C} \,|\, \lambda = \lambda_1\lambda_2,\, \lambda_j \in \sigma(A_j),\, j = 1, 2\}. \end{aligned} \tag{4.64}$$

Thus, one can apply (4.54), (4.55), respectively, (4.56), (4.57). □

Of course, the condition on $W$ in the Hilbert–Schmidt context in Lemma 4.10 is much weaker than condition (4.23) since only finitely many Fourier coefficients $\widehat{W}_k$ of $W$ are in involved in the former, while the stronger condition (4.23) is used to prove the convergence of $\mathcal{K}_J$ in Theorem 4.9.

**Remark 4.11.** More generally, any useful approximation of $H^{(0)}_{\Omega,\mathrm{p}}$ may be employed, not necessarily an eigenfunction expansion or one attached to a Fourier basis. In particular, in the case that $V_\infty$ is not constant in $x_2, \dots, x_d$, one may proceed alternatively by Galerkin approximation to approximate $H^{(0)}_{\Omega,\mathrm{p}}$ as the limit of operators with semi-separable integral kernels corresponding to the (no longer decoupled) truncated operator $H^{(0)}_{\Omega,\mathrm{p},\mathrm{K}}$, in a spirit similar to [23]. Likewise, it is not essential to assume that $V$ has common limits at $x_1 = +\infty$ and $x_1 = -\infty$; one may consider also "front-type" solutions with $\lim_{x_1\to\pm\infty} U(x_1,\,\cdot\,) = U_\pm$, though this introduces some additional technicalities in the analysis connected with invertibility of $H^{(0)}_{\Omega,\mathrm{p}}$.

4.1.4. *Connection with Galerkin-based Evans functions.* At this point, adopting the point of view of [23], we consider $\mathcal{K}_J$ as an operator with a matrix-valued integral kernel, and acting on the subspace $\mathcal{L}_J$ of $L^2\big(\Omega; dy; L^2(\mathbb{R}; dx_1)\big)$ spanned by Fourier modes with wave-number of modulus less than or equal to $J$, that is, on

$$\mathcal{L}_J = \bigg\{ w(x) = \sum_{|m|\leqslant J} \hat w_m(x_1) e^{im\cdot y} \,\bigg|\, \hat w_m \in L^2(\mathbb{R}; dx_1)\bigg\}. \tag{4.65}$$

We let $N_J$ denote the number of these modes. Using Lemma 4.10, one verifies that $\mathcal{K}_J(z) \in \mathcal{B}_2\big(L^2(\mathbb{R}\times\Omega; dx)\big)$ and thus

$$\det{}_{2,L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z)) = \det{}_{2,\mathcal{L}_J}(I_{\mathcal{L}_J} - \mathcal{K}_J(z)) \tag{4.66}$$

is well-defined. Equivalently, since the Fourier modes form an orthonormal basis, and hence the determinant is invariant under the Fourier transform, we compute (on the subspace $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{N_J}\big)$ of $L^2\big(\mathbb{R}; dx_1; \ell^2(\mathbb{Z}^{d-1})\big)$ isomorphic to $\mathcal{L}_J$ via the Fourier transform) instead of (4.35) the Fredholm determinant

$$\det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})} - \widehat{\mathcal{K}}_J(z)\big), \tag{4.67}$$

where $\widehat{\mathcal{K}}_J(z)$ on $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{N_J}\big)$ is defined in terms of its integral kernel

$$\widehat{\mathcal{K}}_J(z, x_1, x_1') = \bigg(\frac{-e^{-(V_\infty+|j|^2-z)^{1/2}|x_1-x_1'|}}{2(V_\infty+|j|^2-z)^{1/2}} \widehat{W}_{j-m}(x_1')\bigg)_{|j|,|m|\leqslant J} \tag{4.68}$$

$$= \begin{cases} F_1(x_1)G_1^\top(x_1'), & x_1' > x_1, \\ F_2(x_1)G_2^\top(x_1'), & x_1 > x_1', \end{cases} \tag{4.69}$$

as an operator with a single, matrix-valued semi-separable integral kernel, where $F_k$ and $G_k$ denote the $N_J \times N_J$ matrices

$$(F_k)_{m,j} = \big(\widehat{f_k^j}\big)_m, \quad (G_k)_{m,j} = \big(\widehat{g_k^j}\big)_{-m}, \quad k = 1, 2, \tag{4.70}$$

and $G_k^\top = ((G_k)_{j,m})$ denotes the transpose of the matrix $G_k = ((G_k)_{m,j})$, $k = 1, 2$.

We briefly pause for a moment and recall the principal underlying idea here: The operator $\mathcal{K}_J$ acts on the space $L^2\big(\mathbb{R}; dx_1; L^2(\Omega; dy)\big)$ and leaves invariant its subspace $\mathcal{L}_J$ which, in fact, is isomorphic to $L^2\big(\mathbb{R}; dx_1; L^2_{N_J}(\Omega; dy)\big)$, where $L^2_{N_J}(\Omega; dy)$ is the subspace of $L^2(\Omega; dy)$ spanned by the $N_J$ exponentials $\{e^{iy\cdot j}\}_{|j|\leqslant J}$. Via the Fourier transform, $L^2_{N_J}(\Omega; dy)$ is isometrically isomorphic to $\mathbb{C}^{N_J}$ viewed as a subspace in $\ell^2(\mathbb{Z}^{d-1})$. Indeed, if $j \in \mathbb{Z}^{d-1}$ and $|j| \leqslant J$, then the Fourier transform maps the element $e^{ij\cdot y}$ of the basis of $L^2(\Omega; dy)$ into the sequence $\delta_j = \{\delta_{m,j}\}_{m\in\mathbb{Z}^{d-1}} \in \ell^2(\mathbb{Z}^{d-1})$. Indexing a basis in $\mathbb{C}^{N_J}$ by means of the indices $j \in \mathbb{Z}^{d-1}$, $|j| \leqslant J$, we fix an isomorphism between $\mathbb{C}^{N_j}$ and the subspace of $\ell^2(\mathbb{Z}^{d-1})$ spanned by $\delta_j$, $|j| \leqslant J$, and thus between $\mathbb{C}^{N_j}$ and $L^2_{N_J}(\Omega; dy)$. Clearly, via the Fourier transform, the operator $\mathcal{K}_J$ on $L^2\big(\mathbb{R}; dx_1; L^2_{N_J}(\Omega; dy)\big)$ then becomes the operator $\widehat{\mathcal{K}}_J$ on $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{N_J}\big)$. In particular, if $\mathcal{K}_J$ (and hence $\widehat{\mathcal{K}}_J$) is also of trace class, then the traces of $\mathcal{K}_J$ and $\widehat{\mathcal{K}}_J$ are equal as will be used below in the proof of the second equality in (4.76). It is the operator $\widehat{\mathcal{K}}_J$ which finally is an operator with a semi-separable integral kernel.

**Remark 4.12.** The vector-valued case $w \in \mathbb{R}^n$ may be treated similarly, with $V_\infty$ now a positive-definite $n \times n$ matrix, and $F_k$, $G_k \in \mathbb{R}^{nN_J \times nN_J}$.

Our objective is to relate the truncated 2-modified Jost function (4.35) and the Evans function for the eigenvalue problem (4.7). We rewrite (4.7) in matrix form as

$$\Big(-\frac{d^2}{dx_1^2} + V_\infty I_{\mathbb{C}^{N_J}} + \mathrm{diag}\,\big\{|j|^2\big\}_{|j|\leqslant J} - zI_{\mathbb{C}^{N_J}} + \mathcal{W}_J\Big)\Psi = 0, \tag{4.71}$$

where $j$ is the Fourier wave number, $|j| \leqslant J$, $\Psi = \Psi(x_1)$ is an $\mathbb{C}^{N_J}$-valued function on $\mathbb{R}$, $\mathrm{diag}\,\big\{|j|^2\big\}_{|j|\leqslant J}$ is a diagonal matrix of dimensions $N_J \times N_J$, and $\mathcal{W}_J + V_\infty I_{\mathbb{C}^{N_J}}$ is the matrix representation of some chosen truncation of the convolution operator $\widehat{V} * \cdot$ . This choice is to be followed consistently in both Galerkin-based and Fredholm computations. Specifically, if $\Psi = (\hat{\psi}_m)_{|m|\leqslant J}$ for the eigenfunction $\psi$ in (4.7), then

$$\mathcal{W}_J(x_1) = \big(\widehat{W}_{j-m}(x_1)\big)_{|j|,|m|\leqslant J}, \quad x_1 \in \mathbb{R}, \tag{4.72}$$

where $\widehat{W}_\ell(x_1)$ are the Fourier coefficients of $W(x_1, \cdot\,) = V(x_1, \cdot\,) - V_\infty$. Introducing the self-adjoint operator $\mathcal{H}_J$ in $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{N_J}\big)$,

$$\mathcal{H}_J = -\frac{d^2}{dx_1^2} + V_\infty I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})} + \mathrm{diag}\,\big\{|j|^2\big\}_{|j|\leqslant J} + \mathcal{W}_J, \quad \mathrm{dom}(\mathcal{H}_J) = H^2\big(\mathbb{R}; \mathbb{C}^{N_J}\big), \tag{4.73}$$

we note that the asymptotic operator for the operator $\mathcal{H}_J$ in (4.73), viewed as a one-dimensional matrix-valued second-order differential operator in $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{N_J}\big)$, is given by

$$\mathcal{H}_J^{(0)} = -\frac{d^2}{dx_1^2} + V_\infty I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})} + \mathrm{diag}\,\big\{|j|^2\big\}_{|j|\leqslant J}, \quad \mathrm{dom}\big(\mathcal{H}_J^{(0)}\big) = H^2\big(\mathbb{R}; \mathbb{C}^{N_J}\big), \tag{4.74}$$

and thus the operator

$$\widehat{\mathcal{K}}_J(z) = -\big(\mathcal{H}_J^{(0)} - zI_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}\big)^{-1}\mathcal{W}_J, \quad z \in \mathbb{C}\backslash\sigma\big(\mathcal{H}_J^{(0)}\big), \tag{4.75}$$

is the Birman–Schwinger-type operator (cf. (4.12)) for the pair of the truncated operators $\mathcal{H}_J$ and $\mathcal{H}_J^{(0)}$.

**Lemma 4.13.** *Let $z \in \mathbb{C}$ such that $z \notin \sigma\big(\mathcal{H}_J^{(0)}\big)$. In addition, assume that $\widehat{W}_{j-m} \in \ell^1\big(L^2(\mathbb{R}; dx_1)\big) \cap C(\mathbb{R})$ for all $m, j \in \mathbb{Z}$, $|m|, |j| \leqslant J$. Then the operator $\widehat{\mathcal{K}}_J(z)$ is of trace class on $L^2(\mathbb{R}; dx_1; \mathbb{C}^{N_J})$, the operator $\mathcal{K}_J(z)$ is of trace class on $L^2(\mathbb{R}\times\Omega; dx)$, their traces are equal and given by the following expression $\Theta_J(z)$:*

$$\Theta_J(z) = \mathrm{tr}_{L^2(\mathbb{R}\times\Omega;dx)}(\mathcal{K}_J(z)) = \mathrm{tr}_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_j})}\big(\widehat{\mathcal{K}}_J(z)\big) \tag{4.76}$$

$$= -\frac{1}{2}\bigg(\int_{\mathbb{R}\times\Omega} dx\, W(x)\bigg) \sum_{|j|\leqslant J} (V_\infty + |j|^2 - z)^{-1/2}. \tag{4.77}$$

*Proof.* By Lemma 4.10 (*ii*), $\mathcal{K}_J(z)$ and each $\mathcal{K}_{m,j}(z)$ in (4.47) is a trace class operator on $L^2(\mathbb{R} \times \Omega; dx)$. In addition, each of the integral kernels of $\mathcal{K}_J(z)$ and $\mathcal{K}_{m,j}(z)$ is continuous on the diagonal. Thus, [2, Corollary 3.2] applies and hence

$$\mathrm{tr}_{L^2(\mathbb{R}\times\Omega;dx)}(\mathcal{K}_J(z)) = \sum_{|m|,|j|\leqslant J} \mathrm{tr}_{L^2(\mathbb{R}\times\Omega;dx)}(\mathcal{K}_{m,j}(z))$$

$$
\begin{aligned}
&= -\frac{1}{2} \sum_{|m|,|j| \leqslant J} \int_{\mathbb{R}} dx_1 \, \widehat{W}_{j-m}(x_1) \frac{1}{(V_\infty + |j|^2 - z)^{1/2}} \int_\Omega dy \, e^{i(j-m)y} \\
&= -\frac{1}{2} \sum_{|m|,|j| \leqslant J} \int_{\mathbb{R}} dx_1 \, \widehat{W}_{j-m}(x_1) \frac{1}{(V_\infty + |j|^2 - z)^{1/2}} \, (2\pi)^{d-1} \delta_{m,j} \\
&= -\frac{1}{2} \bigg( (2\pi)^{d-1} \int_{\mathbb{R}} dx_1 \, \widehat{W}_0(x_1) \bigg) \sum_{|j| \leqslant J} \frac{1}{(V_\infty + |j|^2 - z)^{1/2}} \\
&= -\frac{1}{2} \bigg( \int_{\mathbb{R}\times\Omega} dx \, W(x) \bigg) \sum_{|j| \leqslant J} \frac{1}{(V_\infty + |j|^2 - z)^{1/2}}, \qquad (4.78)
\end{aligned}
$$

proving (4.77).

Finally, denote by $\mathcal{P}_J$ the orthogonal projection in $L^2(\mathbb{R}\times\Omega; dx)$ onto $\mathcal{L}_J$ and by $\mathcal{Q}_J = I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{P}_J$ the complementary projection. Since $\mathcal{L}_J$ is a reducing subspace for $\mathcal{K}_J$,

$$\mathcal{K}_J \mathcal{P}_J = \mathcal{P}_J \mathcal{K}_J, \qquad (4.79)$$

one can write $\mathcal{K}_J$ in $L^2(\mathbb{R}\times\Omega; dx)$ in terms of the $2\times 2$ block decomposition

$$\mathcal{K}_J(z) = \begin{pmatrix} \mathcal{K}_J\big|_{\operatorname{ran}(\mathcal{P}_J)}(z) & 0 \\ 0 & 0 \end{pmatrix} \qquad (4.80)$$

with respect to the decomposition

$$
\begin{aligned}
L^2(\mathbb{R}\times\Omega; dx) &= \mathcal{P}_J L^2(\mathbb{R}\times\Omega; dx) \oplus \mathcal{Q}_J L^2(\mathbb{R}\times\Omega; dx) \\
&= \mathcal{L}_J \oplus \mathcal{Q}_J L^2(\mathbb{R}\times\Omega; dx).
\end{aligned} \qquad (4.81)
$$

Since $\mathcal{K}_J\big|_{\operatorname{ran}(\mathcal{P}_J)}$ is unitarily equivalent to $\widehat{K}_J(z)$ via the Fourier transform, (4.80) implies that $\mathcal{K}_J(z)$ and $\widehat{\mathcal{K}}_J(z)$ are trace class operators at the same time, and it also implies equality of the following traces:

$$
\begin{aligned}
\operatorname{tr}_{L^2(\mathbb{R}\times\Omega;dx)}(\mathcal{K}_J(z)) &= \operatorname{tr}_{\mathcal{L}_J}\Big(\mathcal{K}_J\big|_{\operatorname{ran}(\mathcal{P}_J)}(z)\Big) \\
&= \operatorname{tr}_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}\big(\widehat{\mathcal{K}}_J(z)\big),
\end{aligned} \qquad (4.82)
$$

proving the second equality in (4.76). □

**Remark 4.14.** We emphasize that the sequence $\{\Theta_J(z)\}_{J\geqslant 0}$ diverges as $J\to\infty$ for $d \geqslant 2$. The latter fact does not permit us to use in the subsequent analysis the non-modified Jost function $\mathcal{F}_J(z) = \det_{L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z))$ and pass in (4.93) to the limit as $J\to\infty$; instead, it forces us to work with the 2-modified Jost function $\mathcal{F}_{2,J}(z)$ defined in (4.35).

Denote by $\mathcal{E}_J$ the Evans functions for the one-dimensional approximate system (4.7) obtained by Galerkin approximation/Fourier truncation at the level $|j| \leqslant J$, for simplicity of discussion normalized as described in [11] to agree with the corresponding (one-dimensional) 2-modified Fredholm determinant. Following the approach of [11], we recall that the Evans function $\mathcal{E}_J(z)$ is defined as a $2N_J \times 2N_J$ Wronskian

$$\mathcal{E}_J(z) = \det(\mathcal{Y}) = \det(\mathcal{Y}_1^+, \dots, \mathcal{Y}_{2N_J}^-), \qquad (4.83)$$

where the $(2N_J \times 1)$-vectors $\mathcal{Y}_1^+, \dots, \mathcal{Y}_{2N_J}^-$ are bases of solutions decaying at $x_1 = +\infty$, respectively, at $x_1 = -\infty$, of the first-order system equivalent to the second-order differential equation (4.71), lying in appropriately prescribed directions at spatial infinity. The solutions are chosen in [11] in a way that $\mathcal{E}_J$ does not depend on the choice of coordinate system in $\mathbb{C}^{2N_J}$ and does not change under similarity transformations of the system. Specifically, let us introduce the $(2N_J \times 2N_J)$ matrices

$$\mathcal{A} = \begin{pmatrix} 0 & I_{\mathbb{C}^{N_J}} \\ h & 0 \end{pmatrix}, \quad R(x_1) = \begin{pmatrix} 0 & 0 \\ \mathcal{W}_J(x_1) & 0 \end{pmatrix}, \quad x_1 \in \mathbb{R}, \tag{4.84}$$

where, for brevity, we denote

$$h(z) = (V_\infty - z) I_{\mathbb{C}^{N_J}} + \operatorname{diag}\big\{|j|^2\big\}_{|j|\leqslant J}. \tag{4.85}$$

Now $d\mathcal{Y}/dx_1 = (\mathcal{A} + R(x_1))\mathcal{Y}$ is the first-order system equivalent to the second-order differential equation (4.71). We introduce on the space $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{2N_J}\big)$ the first order differential operators $G_J^{(0)} = (d/dx_1) - \mathcal{A}$ and $G_J = (d/dx_1) - \mathcal{A} - R(x_1)$ and the respective Birman–Schwinger-type integral operator

$$\widetilde{\mathcal{K}}_J(z) = -((d/dx_1) - \mathcal{A})^{-1} R(x_1). \tag{4.86}$$

According to the main result in [11], the Evans function $\mathcal{E}_J(z)$ is equal (up to the explicitly computed factor $e^{-\Theta_J(z)}$, that is non degenerate and analytic with respect to $z$) to the 2-modified Fredholm determinant of the operator $I_{L^2(\mathbb{R}; dx_1; \mathbb{C}^{2N_J})} - \widetilde{\mathcal{K}}_J(z)$ on $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{2N_J}\big)$ corresponding to the first-order system mentioned above. As we will see next (cf. also [13, Theorem 4.7]), this 2-modified Fredholm determinant is equal to the 2-modified Fredholm determinant of the operator $I_{L^2(\mathbb{R}; dx_1; \mathbb{C}^{N_J})} - \widehat{\mathcal{K}}(z)$ on $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{N_J}\big)$ corresponding to the second-order operator $\mathcal{H}_J$ in (4.71). Thus, we obtain evidently that the Evans function $\mathcal{E}_J$ coincides with the following (non-modified(!)) Fredholm determinant (that is, with the Jost function):

$$\mathcal{F}_J(z) = \det_{L^2(\mathbb{R}; dx_1; \mathbb{C}^{N_J})}\Big(I_{L^2(\mathbb{R}; dx_1; \mathbb{C}^{N_J})} + \big(\mathcal{H}_J^{(0)} - z I_{L^2(\mathbb{R}; dx_1; \mathbb{C}^{N_J})}\big)^{-1} \mathcal{W}_J\Big). \tag{4.87}$$

Thus, we have the following main result, extending the one-dimensional theory of [11]. One of its main points can be explained as follows: Zeros of the Evans function $\mathcal{E}_J$ or, equivalently, of the Jost function $\mathcal{F}_J$, are the eigenvalues of the operator $\mathcal{H}_J$. The eigenvalues are also zeros of the 2-modified Fredholm determinant $\mathcal{F}_{2,J}$. The modified and nonmodified determinants are equal up to the nonzero exponential factor $e^{\Theta_J}$, where $\Theta_J$ is the trace described in (4.77). From this point of view the use of the nonmodified determinant $\mathcal{F}_J$ (or $\mathcal{E}_J$) and the 2-modified determinant $\mathcal{F}_{2,J}$ are equivalent, as far as finding the eigenvalues of $\mathcal{H}_J$ is concerned. However, the nonmodified determinants have an advantage because the sequence $\{\mathcal{F}_{2,J}\}$ converges to $\mathcal{F}_2$ as $J \to \infty$, while the sequences $\{\mathcal{F}_J\}$, $\{\mathcal{E}_J\}$, and $\{\Theta_J\}$, all diverge. Thus, for the truncated problem, the use of the 2-modified Fredholm determinants appears to be more natural than the use of the Evans function.

**Theorem 4.15.** *Let $z \in \mathbb{C}$ such that $z \notin \sigma\big(\mathcal{H}_J^{(0)}\big)$ and assume that $\widehat{W}_{j-m} \in \ell^1\big(L^2(\mathbb{R}; dx_1)\big) \cap C(\mathbb{R})$ for all $m, j \in \mathbb{Z}$, $|m|, |j| \leqslant J$. Then the Galerkin-based Evans function $\mathcal{E}_J(z)$, the Jost function $\mathcal{F}_J(z) = \det_{L^2(\mathbb{R}\times\Omega; dx)}(I_{L^2(\mathbb{R}\times\Omega; dx)} - \mathcal{K}_J(z))$, and the approximate modified Fredholm determinants for the operators in* (4.75) *and* (4.86) *are related as follows:*

$$\mathcal{F}_{2,J}(z) = \det_{2, L^2(\mathbb{R}\times\Omega; dx)}(I_{L^2(\mathbb{R}\times\Omega; dx)} - \mathcal{K}_J(z)) \tag{4.88}$$

$$= \det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})} - \widetilde{\mathcal{K}}_J(z)\big) \tag{4.89}$$
$$= e^{\Theta_J(z)}\mathcal{E}_J(z) \tag{4.90}$$
$$= e^{\Theta_J(z)}\det{}_{L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z)) \tag{4.91}$$
$$= e^{\Theta_J(z)}\mathcal{F}_J(z), \tag{4.92}$$

*where $\Theta_J(z)$ is the trace of the operator $\mathcal{K}_J(z)$ given in formula (4.77).*

*Proof.* Since $\mathcal{K}_J(z)$ is of trace class on $L^2(\mathbb{R}\times\Omega; dx)$, $\Theta_J(z)$ is the trace of $\mathcal{K}_J(z)$, and $\mathcal{F}_J(z)$ is just a notation for $\det_{L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z))$, the equality of (4.88), (4.91) and (4.92) trivially follows from (cf. (2.41))

$$\begin{aligned}&\det{}_{2,L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z))\\ &\quad = \det{}_{L^2(\mathbb{R}\times\Omega;dx)}(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z))e^{\operatorname{tr}_{L^2(\mathbb{R}\times\Omega;dx)}(\mathcal{K}_J(z))}.\end{aligned} \tag{4.93}$$

To show that the modified Fredholm determinants in (4.88) and (4.89) are equal, we will utilize an idea from the proof of [22, Proposition 8.1] (see also a related result in [13, Theorem 4.7]). We introduce the following operator matrices acting on $L^2\big(\mathbb{R}; dx_1; \mathbb{C}^{2N_J}\big)$:

$$T = 2^{-1/2}\begin{pmatrix} h^{1/2} & -I \\ h^{1/2} & I \end{pmatrix}, \quad T^{-1} = 2^{-1/2}\begin{pmatrix} h^{-1/2} & h^{-1/2} \\ -I & I \end{pmatrix}, \tag{4.94}$$
$$E = \begin{pmatrix} -I & -I \\ I & I \end{pmatrix}, \quad Q = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \tag{4.95}$$

where $I = I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}$ and $h$ is defined in (4.85). In addition, we use the related similarity transformation in (4.84) and (4.86) to define the following matrices and operators

$$\mathcal{A}^{(1)} = T\mathcal{A}T^{-1}, \quad R^{(1)}(x_1) = TR(x_1)T^{-1}, \quad \widetilde{\mathcal{K}}_J^{(1)}(z) = T\widetilde{\mathcal{K}}_J(z)T^{-1}. \tag{4.96}$$

A short calculation reveals:

$$\mathcal{A}^{(1)} = \operatorname{diag}\big\{-h^{1/2}, h^{1/2}\big\}, \tag{4.97}$$
$$R^{(1)}(x_1) = 2^{-1}\mathcal{W}_J E h^{-1/2}, \tag{4.98}$$
$$\widetilde{\mathcal{K}}_J^{(1)}(z) = 2^{-1}\begin{pmatrix} -((d/dx_1) + h^{1/2})^{-1}\mathcal{W}_J \\ ((d/dx_1) - h^{1/2})^{-1}\mathcal{W}_J \end{pmatrix}\begin{pmatrix} h^{-1/2} & h^{-1/2}\end{pmatrix}. \tag{4.99}$$

Changing the order of multiplication of the operators blocks in (4.99), one infers

$$2^{-1}\begin{pmatrix} h^{-1/2} & h^{-1/2}\end{pmatrix}\begin{pmatrix} -((d/dx_1) + h^{1/2})^{-1}\mathcal{W}_J \\ ((d/dx_1) - h^{1/2})^{-1}\mathcal{W}_J \end{pmatrix} = \big((d^2/dx_1^2) - h\big)^{-1}\mathcal{W}_J. \tag{4.100}$$

Thus, using the standard determinant property (2.2) and recalling (4.75), we conclude that (4.88) and (4.89) are equal,

$$\begin{aligned}&\det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})} - \widetilde{\mathcal{K}}_J(z)\big)\\ &\quad = \det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})} - \widetilde{\mathcal{K}}_J^{(1)}(z)\big)\\ &\quad = \det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})} - ((d^2/d^2x_1^2) - h)^{-1}\mathcal{W}_J\big)\\ &\quad = \det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}\Big(I + \big(\mathcal{H}_J^{(0)} - zI\big)^{-1}\mathcal{W}_J\Big)\\ &\quad = \det{}_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{N_J})} - \widehat{\mathcal{K}}_J(z)\big)\end{aligned}$$

$$= \det_{2,L^2(\mathbb{R}\times\Omega;dx)}\big(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_J(z)\big). \tag{4.101}$$

Finally, to show that (4.89) and (4.90) are equal, we apply the similarity transformation (4.96) and replace the differential equation $d\mathcal{Y}/dx_1 = (\mathcal{A} + R(x_1))\mathcal{Y}$ by $d\mathcal{Y}/dx_1 = (\mathcal{A}^{(1)} + R^{(1)}(x_1))\mathcal{Y}$. We will now use one of the main results of [11]. Since the real part of the spectrum of $h^{1/2}$ (for $h$ defined in (4.85)) is positive due to our convention $\operatorname{Im}(z) \geqslant 0$, the unperturbed equation $d\mathcal{Y}/dx_1 = \mathcal{A}^{(1)}\mathcal{Y}$, due to (4.97), has the exponential dichotomy on $\mathbb{R}$ with the dichotomy projection $Q$ defined in (4.95). Therefore, according to [11, Theorem 8.37], under assumption (4.13) we have the formula

$$\det_{2,L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})}\big(I_{L^2(\mathbb{R};dx_1;\mathbb{C}^{2N_J})} - \widetilde{\mathcal{K}}_J^{(1)}(z)\big) = e^{\widetilde{\Theta}_J(z)}\mathcal{E}_J(z), \tag{4.102}$$

where $\widetilde{\Theta}_J(z)$ is defined as follows:

$$\widetilde{\Theta}_J(z) = \int_0^\infty dx_1 \operatorname{tr}_{\mathbb{C}^{2N_J}}\big[QR^{(1)}(x_1)\big] - \int_{-\infty}^0 dx_1 \operatorname{tr}_{\mathbb{C}^{2N_J}}\big[(I_{\mathbb{C}^{2N_J}} - Q)R^{(1)}(x_1)\big]. \tag{4.103}$$

Using (4.95) and (4.98), it follows that $\widetilde{\Theta}_J(z) = \Theta_J(z)$, completing the proof. □

**Remark 4.16.** We have a similar result in the vector-valued case mentioned in Remark 4.12 also in the front-type setting discussed in Remark 4.11.

4.1.5. *Alternative computation.* For its own interest, and for reference in the following subsections, we mention an alternative method of computing $\mathcal{F}_{2,J}$ directly from the reduction of [13], where the Jost function has been computed, without carrying out the full analysis of [11] relating this to the Evans function. Comparing (4.69), and [13, (1.17)] with $\alpha = 1$, we have the following representation:

$$\mathcal{F}_{2,J}(z) = \det_{2,\mathbb{C}^{N_J}}\left(I_{\mathbb{C}^{N_J}} - \int_{\mathbb{R}^2} dx_1\, dx_1'\, G_2(x_1)\big(I_{\mathbb{C}^{2N_J}} + \mathcal{J}(x_1,x_1')\big)F_2(x_1')\right), \tag{4.104}$$

where

$$\mathcal{J}(x_1,x_1') = C(x_1)\mathcal{U}(x_1)^{-1}\mathcal{U}(x_1')B(x_1'), \tag{4.105}$$

$$B = \begin{pmatrix} G_1^\top & -G_2^\top \end{pmatrix}^\top, \quad C = \begin{pmatrix} F_1 & F_2 \end{pmatrix}, \tag{4.106}$$

$$A = \begin{pmatrix} G_1^\top F_1 & G_1^\top F_2 \\ -G_2^\top F_1 & -G_2^\top F_2 \end{pmatrix}, \tag{4.107}$$

and $\mathcal{U}$ is any nonsingular solution of the first-order system

$$\frac{d\mathcal{U}(x_1)}{dx_1} = A(x_1)\mathcal{U}(x_1). \tag{4.108}$$

The formulation (4.108) is not numerically useful, since the off-diagonal elements of $A$ are exponentially growing with rate of order $e^{J|x_1|}$. However, noting that $G_{1,2}^\top(x_1')$, respectively, $F_{1,2}(x_1)$ factor as $\operatorname{diag}\big\{e^{\mp(V_\infty+|j|^2-z)^{1/2}x_1'}\mathcal{W}_J\big\}$, respectively, $\operatorname{diag}\big\{(V_\infty+|j|^2-z)^{-1/2}e^{\pm(V_\infty+|j|^2-z)^{1/2}x_1}\big\}$, we may reduce (4.108) by the coordinate change $\mathcal{V} = D\mathcal{U}$, with

$$D = \operatorname{diag}\left\{\frac{e^{(V_\infty+|j|^2-z)^{1/2}x_1}}{(V_\infty+|j|^2-z)^{1/2}}, \frac{e^{-(V_\infty+|j|^2-z)^{1/2}x_1}}{(V_\infty+|j|^2-z)^{1/2}}\right\}, \tag{4.109}$$

to a bounded-coefficient system (cf. (4.85)),

$$\begin{aligned} &\frac{d\mathcal{V}(x_1)}{dx_1} = A_b(x_1)\mathcal{V}(x_1), \\ &A_b(x_1) = \begin{pmatrix} h^{1/2} + h^{-1/2}\mathcal{W}_J(x_1) & h^{-1/2}\mathcal{W}_J(x_1) \\ -h^{-1/2}\mathcal{W}_J(x_1) & -h^{1/2} - h^{-1/2}\mathcal{W}_J(x_1) \end{pmatrix}, \end{aligned} \tag{4.110}$$

of a form readily solved by the same techniques used to solve the first-order eigenvalue ODE for basis solutions $\mathcal{Y}_\ell$ in (4.83). Indeed, this can be recognized as essentially the same ODE.

**Remark 4.17.** Likewise, one might start with the Evans formulation (4.71), written as a first order system, and try to precondition by factoring out the expected asymptotic behavior, to obtain essentially system (4.108). That is, the operations of preconditioning (viewing the Fredholm formulation as an analogous preconditioning step of factoring out expected spatially-asypmptotic behavior) and reduction to ODE essentially commute, at least in this simple case.

4.1.6. *Stability index computation.* Following the approach of Section 4.1.5, computation of the multi-dimensional stability index can be carried out in the same way, with no additional complications. For, exactly as in (3.64) of the one-dimensional case (but using (2.52)), one has the formula

$$\mathcal{F}_2^\bullet(0) = \det_{2,L^2(\mathbb{R}\times\Omega;dx)}\big(I_{L^2(\mathbb{R}\times\Omega;dx)} - \mathcal{K}_0 - P_0\big)\det_{P_0L^2(\mathbb{R}\times\Omega;dx)}(P_0\mathcal{K}_1P_0), \tag{4.111}$$

with $\mathcal{K}_0 = \mathcal{K}(0) = -\overline{H_{\Omega,\mathrm{p}}^{(0)}{}^{-1}uv}$ and $\mathcal{K}_1 = \mathcal{K}^\bullet(z)\big|_{z=0} = -\overline{H_{\Omega,\mathrm{p}}^{(0)}{}^{-2}uv}$. (One can remove the closure symbols in the last two expressions since all operators involved are bounded.)

The second inner-product-type factor is straightforward to evaluate, requiring only approximation of the eigenfunctions of the operator $I - \mathcal{K}_0$ and its adjoint corresponding to the zero eigenvalue, which in many cases are known from the outset. We recall that in the present case, the eigenfunction $\Phi$ of the operator $I - \mathcal{K}_0$ is $dU/dx_1$; here $U$ is the standing wave, see Section 4.1.1. The eigenfunction $\widetilde{\Phi}$ of the operator $(I - \mathcal{K}_0)^*$ may be deduced by the fact that the original differential operator $L$ is self-adjoint; specifically, $\Big(I - \big(H_{\Omega,\mathrm{p}}^{(0)}\big)^{-1}(V - V_\infty)\Big)\Phi = 0$ implies, by self-adjointness of $\Big(I + \big(H_{\Omega,\mathrm{p}}^{(0)}\big)^{-1}\Big)$ and $(V - V_\infty)$, that $\widetilde{\Phi} = H_{\Omega,\mathrm{p}}^{(0)}\Phi$ is indeed the required eigenfunction: $\Big(I + \big(H_{\Omega,\mathrm{p}}^{(0)}\big)^{-1}(V - V_\infty)\Big)^*\widetilde{\Phi} = 0$.

The first factor in (4.111) on the other hand is the characteristic determinant of a rank-one perturbation at $z = 0$, so can be approximated as in Section 4.1.5 using Galerkin approximation/semi-separable reduction by a finite dimensional determinant. Precisely, combining the steps of Sections 4.1.2 and 4.1.5, one reduces the computation at the $J$-th Galerkin level to the evaluation of a $2(N_J+1)\times 2(N_J+1)$ determinant, obtained by solving a $2(N_J+1)\times 2(N_J+1)$ ODE system

$$\frac{d\widetilde{\mathcal{U}}(x_1)}{dx_1} = \widetilde{A}(x_1)\widetilde{\mathcal{U}}(x_1), \quad \widetilde{\mathcal{U}}(x_1) \in \mathbb{C}^{2(N_J+1)\times 2(N_J+1)}, \tag{4.112}$$

where, similarly to (4.108),

$$\begin{aligned} \widetilde{A} &= \begin{pmatrix} \widetilde{G}_1^\top \widetilde{F}_1 & \widetilde{G}_1^\top \widetilde{F}_2 \\ -\widetilde{G}_2^\top \widetilde{F}_1 & -\widetilde{G}_2^\top \widetilde{F}_2 \end{pmatrix}, \\ \widetilde{F}_k &= \begin{pmatrix} F_k & \Phi \end{pmatrix}, \quad \widetilde{G}_k = \begin{pmatrix} G_k & H^{(0)}_{\Omega,\mathrm{p}} \Phi \end{pmatrix}, \end{aligned} \tag{4.113}$$

and $\Phi$ is the eigenfunction of the operator $\mathcal{K}_0$ corresponding to the eigenvalue 1, that is, $\mathcal{K}_0\Phi = \Phi$. Making the change of coordinates $\widetilde{\mathcal{U}} = \widetilde{D}\widetilde{\mathcal{V}}$, $\widetilde{D} = \operatorname{diag}\{D, 1\}$, see (4.109), we obtain a system $d\widetilde{\mathcal{V}}(x_1)/dx_1 = \widetilde{A}_b(x_1)\widetilde{\mathcal{V}}(x_1)$ with bounded coefficient matrix $\widetilde{A}_b$ that can be numerically solved by standard techniques used to compute the Evans function.

By comparison, if one follows the existing Galerkin methods, working with an approximate truncated system at level $J$, one must face the difficulty that zero eigenvalues for the exact system perturb to small but in general nonzero eigenvalues of the approximate system, making difficult a straightforward numerical computation without further analytical preparations. On the other hand, the usual analytic preparations (see [1],[30]) involve solving variational equations about the zero-energy eigenfunction and also projecting out the zero eigenmodes from other modes to obtain a well-conditioned basis. These do not appear to be real obstructions to the computation, but are at least complications. Perhaps for this reason, to our knowledge no such computation has so far been carried out, or even proposed in full detail.[3]

The formulation of the above multi-dimensional stability index algorithm we thus view as a useful practical contribution of the present work, and its numerical realization as an important direction for further investigation.

4.1.7. *Numerical conditioning.* Last, we examine the question of numerical conditioning. By Theorem 4.15, one way to compute the approximate Fredholm determinants $\mathcal{F}_{2,J}$ is to carry out a standard Evans function computation as in [23]. However, from a numerical perspective, this might be missing the point. For, note that the principal, constant-coefficient diagonal, part of the coefficient matrix of (4.71) has entries $|j|^2$ leading to spatial growth rates $\pm|j|$ of order up to $J$. Computing the Evans function thus involves solution of an ODE that becomes infinitely stiff as $J \to \infty$.

We suggest as a possible alternative, discretizing the kernel $\mathcal{K}_J$ in variables $x_1$, $x_1'$ and directly evaluating the determinant of the resulting $MN_J \times MN_J$ matrix, where $M$ is the number of mesh points in the $x_1$ ($x_1'$) discretization required to give a desired error bound. Noting that $M$ is essentially dimension-independent for simple first-order quadrature (since matrix norm $|\mathcal{W}_J|$ is bounded, by Parseval's identity, while the first derivative of $\operatorname{diag}\left\{\frac{e^{-(V_\infty+|j|^2-z)^{1/2}|x_1|}}{(V_\infty+|j|^2-z)^{1/2}}\right\}$ is of order one), we see that there should be a break-even point at which the cost of order $(MN_J)^3$ of evaluating the discretized determinant should be better than the cost $\sim \tilde{N}(J)N_J^3$ of evaluating the Evans function, or, equivalently,

$$\tilde{N}(J) \geqslant M^3, \tag{4.114}$$

where $\tilde{N}(J)$ denotes the number of mesh points required to evaluate the $2N_J \times 2N_J$ Evans ODE to the same tolerance. For a first-order A-stable scheme, $\tilde{N}(J) \sim MJ^2$

[3]However, see the interesting analysis [28] in the somewhat different spatially periodic case.

(note: this is determined by truncation error, which is estimated as proportional to second derivative of the solution as the square of the norm of the largest eigenvalues $\pm J$), yielding break-even at $J \sim M$, where typical values of $M$ are of order $\sim 100$ [18].

Though hardly conclusive, this rough calculation suggests at least that direct Fredholm computation is worthy of further study; we recall that $J \sim 100$ is the order studied in [23]. Alternatively, one might compute the Evans function not by shooting, but by continuation-type algorithms as suggested by Sandstede [34], viewing the eigenvalue equation as a two-point boundary-value problem, avoiding stiffness by another route; however, so far as we know, such a scheme has not yet been implemented. See [18] for further discussion of this approach.

4.2. **Functions with radial limits.** Finally, consider standing-wave solutions $U$ of (4.1) on the whole space $\mathbb{R}^d$, possessing radial limits in the following sense: Introduce spherical coordinates $x = (r, \omega)$, $r > 0$, $\omega \in S^{d-1}$, and let $U(R, \omega)$, be the restriction of $U$ to the sphere of radius $R$. Then considered as a function of the angle $\omega \in S^{d-1}$, $U(R, \cdot)$, has an $L^1(S^{d-1}; d\omega_{d-1})$-limit as $R \to +\infty$.

**Remark 4.18.** Assuming the hypotheses of Subsection 4.1, there exist radially symmetric solutions $U(|\cdot|)$, where $U$ is the solution of the corresponding one-dimensional problem with the second derivative replaced by the spherical Laplacian. Linearizing about $U$ and expanding in spherical harmonics, one obtains a decoupled family of one-dimensional eigenvalue problems, similarly as in Remark 4.1, each of which possess a well-defined Evans function and stability index. In this case, there is no zero-eigenvalue at the zeroth harmonic (constant function), but there is a zero-eigenvalue of order $d$ at the level of the first harmonic, with associated eigenfunctions $dU(|\cdot|)/dx_j$, $j = 1, \dots, d$, corresponding to translation-invariance of the underlying equations. These may be treated similarly as in Remark 4.1. (However, we note that this involves an Evans function on the half-line $[0, +\infty)$, which involves some modifications and will be analyzed elsewhere.)

**Remark 4.19.** In the general case, Galerkin approximation in spherical harmonics yields a finite-dimensional system for which an Evans function and stability can again be defined, similarly as in Remark 4.3.

4.2.1. *Fredholm determinant version: radial case.* In the simplest situation that $U$ has a single limit as $|x| \to +\infty$, the operator $H^{(0)}_{\Omega,\mathrm{p}}$ is again constant-coefficient, and the procedure of Section 4.1.2 leads again to expansion of $H^{(0)}_{\Omega,\mathrm{p}}$ in a countable sum of operators with semi-separable integral kernels corresponding to the restrictions to different spherical harmonics. In the general case, we may proceed instead by Galerkin approximation as described in Remark 4.11.

**Remark 4.20.** The common feature of the problems discussed is the presence of a single unbounded spatial dimension (axial for cylindrical case, radial for the radial case), along which the semi-separable reduction is performed. In principle, one could treat still more general problems by truncation/disretization of a continuous Fourier integral. In this setting, the reference to a concrete object in the form of a Fredholm determinant might become still more useful for numerical validation/conditioning, as compared to ad hoc constructions like those in Remarks 4.1 and 4.3. However, it is not clear that there would be a computation advantage to doing so.

4.3. **General operators.** We recall from [11], that it was necessary for general first-order operators to relate the Evans function and a 2-modified determinant already in the one-dimensional case, since the Birman–Schwinger kernel is for first-order operators only Hilbert–Schmidt (indeed, this is one of the key insights of [11]). Likewise, for more general operators involving a first-order component, in particular those arising in the study of stability of viscous shock solutions of hyperbolic–parabolic conservation laws appearing in continuum mechanics [47], it is necessary in dimensions $d = 2$ and 3 to relate the Evans function to a higher modified Fredholm determinant, since the Birman–Schwinger kernel is no longer Hilbert–Schmidt. Flow in a cylindrical duct has been studied for viscous shock and detonation waves in [40], [41].

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