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Resolvent expansions for the Schrödinger operator on the discrete half-line

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Simplified models of transport in mesoscopic systems are often based on a small sample connected to a finite number of leads. The leads are often modelled using the Laplacian on the discrete half-line $\mathbb{N}$. Detailed studies of the transport near thresholds require detailed information on the resolvent of the Laplacian on the discrete half-line. This paper presents a complete study of threshold resonance states and resolvent expansions at a threshold for the Schrödinger operator on the discrete half-line $\mathbb{N}$ with a general boundary condition. A precise description of the expansion coefficients reveals their exact correspondence to the generalized eigenspaces, or the threshold types. The presentation of the paper is adapted from that of Ito-Jensen [Rev. Math. Phys. **27** (2015), 1550002 (45 pages)], implementing the expansion scheme of Jensen-Nenciu [Rev. Math. Phys. **13** (2001), 717–754, **16** (2004), 675–677] in its full generality.

I. INTRODUCTION

Simplified models of transport in mesoscopic systems are often based on a small sample connected to a finite number of leads. The leads are often modelled using the Laplacian on the discrete half-line $\mathbb{N}$. Detailed studies of the transport near thresholds require detailed information on the resolvent of the Laplacian on the discrete half-line. For an example see Cornean-Jensen-Nenciu[1] and references therein. The results in this paper allow one to obtain more detailed information on the adiabatic limit studied in Cornean-Jensen-Nenciu[1].

Let H_0 be the positive Laplacian on the discrete half-line $\mathbb{N} = \{1, 2, \ldots\}$, i.e., for any sequence $x\colon \mathbb{N} \to \mathbb{C}$ we define the sequence $H_0 x\colon \mathbb{N} \to \mathbb{C}$ by

$$(H_0 x)[n] = -(x[n+1] + x[n-1] - 2x[n]). \tag{I.1}$$

The definition (I.1) is incomplete without assigning a *boundary condition*, or a *boundary value* $x[0]$ for each sequence $x\colon \mathbb{N} \to \mathbb{C}$. In this paper we focus on the *Dirichlet boundary condition*:

$$x[0] = 0. \tag{I.2}$$

In other words, we set for any sequence $x\colon \mathbb{N} \to \mathbb{C}$

$$(H_0 x)[n] = \begin{cases} 2x[1] - x[2] & \text{for } n = 1, \\ 2x[n] - x[n+1] - x[n-1] & \text{for } n \geq 2. \end{cases} \tag{I.3}$$

The restriction of H_0 to the Hilbert space $\mathcal{H} = \ell^2(\mathbb{N})$ is bounded and self-adjoint, and its spectrum is

$$\sigma(H_0) = \sigma_{\mathrm{ac}}(H_0) = [0, 4]. \tag{I.4}$$

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The points $0, 4 \in \sigma(H_0)$ are called the *thresholds*. The purpose of this paper is to analyze the threshold behavior of a perturbed Laplacian $H = H_0 + V$ on the discrete half-line $\mathbb{N}$. We compute an asymptotic expansion of the resolvent $R(z) = (H - z)^{-1}$ at the threshold $z = 0$, and, in particular, describe a precise relation between the expansion coefficients and the generalized eigenspaces. The generalized eigenspace considered here is the largest possible one, and includes the threshold resonance states as a part of it. These investigations are done in the same manner as in Ito-Jensen[2], employing the expansion scheme given in Jensen-Nenciu[3,4]. The technique used in Ito-Jensen[2] to treat the threshold 4 can be applied here. Hence we discuss only the threshold zero.

The starting point of our analysis is the free resolvent kernel discussed in Section II. The main results of the paper will be presented in Section III. Actually general boundary conditions are included in our setting as specific forms of perturbations of the Dirichlet Laplacian. We will see this in Section IV. Section V is devoted to an analysis of the generalized eigenspace. After a short preliminary presentation in Section VI, the proofs of the main theorems will be provided in Sections VII–X according to each threshold type. There we will repeatedly use the inversion formula from Jensen-Nenciu[3], adapted to the case at hand. As a reference we will quote the formula in the form given in Ito-Jensen[2] in Appendix A.

There is a large number of papers on discrete Schrödinger operators. However, as far as we are aware, the complete threshold analyses and the resolvent expansions presented here are new.

II. THE FREE LAPLACIAN

In this section we discuss properties of the free Dirichlet Laplacian H_0 on the discrete half-line $\mathbb{N}$ defined by (I.1) and (I.2), or by (I.3). The properties presented here may be considered as a prototype of our main results for a perturbed Laplacian. They will be employed repeatedly both in stating and in proving the main theorems.

Let $\widehat{\mathcal{H}} = L^2(0, \pi)$, and define the Fourier transform $\mathcal{F}\colon \mathcal{H} \to \widehat{\mathcal{H}}$ and its inverse $\mathcal{F}^*\colon \widehat{\mathcal{H}} \to \mathcal{H}$ by

$$(\mathcal{F}x)(\theta) = \sqrt{2/\pi} \sum_{n=1}^{\infty} x[n] \sin(n\theta),$$

$$(\mathcal{F}^* f)[n] = \sqrt{2/\pi} \int_0^{\pi} f(\theta) \sin(n\theta)\, d\theta.$$

Then we have a spectral representation of H_0:

$$\mathcal{F} H_0 \mathcal{F}^* = 2 - 2\cos\theta = 4\sin^2(\theta/2). \tag{II.1}$$

This in fact verifies (I.4). Using the expression (II.1), or antisymmetrizing the kernel of resolvent on the whole line $\mathbb{Z}$, see e.g. Ito-Jensen[2], we can compute the kernel of resolvent $R_0(z) = (H_0 - z)^{-1}$: For $z \in \mathbb{C} \setminus [0, 4]$ with $z \sim 0$ we have

$$R_0(z)[n, m] = \frac{i}{2\sin\phi}\bigl(e^{i\phi|n-m|} - e^{i\phi(n+m)}\bigr), \quad n, m \in \mathbb{N}. \tag{II.2}$$

Here the variable $z \in \mathbb{C} \setminus [0, 4]$ is related to ϕ through the correspondence

$$z = 4\sin^2(\phi/2), \quad \operatorname{Im}\phi > 0.$$

Using the expression (II.2), we can explicitly compute the expansion of $R_0(z)$ around $z = 0$. Before stating it let us introduce the notation employed in this paper.

Notation. In expansions we change variable from $z \in \mathbb{C} \setminus [0, \infty)$ to κ. These variables are related as

$$\kappa = -i\sqrt{z}, \quad \operatorname{Im} z > 0, \quad \operatorname{Im}\sqrt{z} > 0. \tag{II.3}$$

We freely write $R(z)$ as $R(\kappa)$, etc. We use the notation

$$n \wedge m = \min\{n, m\}, \quad n \vee m = \max\{n, m\}.$$

For $s \in \mathbb{R}$ we let

$$\begin{aligned}
\mathcal{L}^s &= \ell^{1,s}(\mathbb{N}) \\
&= \Big\{x \colon \mathbb{N} \to \mathbb{C}; \\
&\qquad \|x\|_{1,s} = \sum_{n\in\mathbb{N}} (1+n^2)^{s/2}|x[n]| < \infty\Big\}, \\
(\mathcal{L}^s)^* &= \ell^{\infty,-s}(\mathbb{N}) \\
&= \Big\{x \colon \mathbb{N} \to \mathbb{C}; \\
&\qquad \|x\|_{\infty,-s} = \sup_{n\in\mathbb{N}} (1+n^2)^{-s/2}|x[n]| < \infty\Big\}.
\end{aligned}$$

We denote the set of all bounded operators from a general Banach space $\mathcal{K}$ to another $\mathcal{K}'$ by $\mathcal{B}(\mathcal{K}, \mathcal{K}')$, and abbreviate $\mathcal{B}(\mathcal{K}) = \mathcal{B}(\mathcal{K}, \mathcal{K})$. In particular, we write

$$\mathcal{B}^s = \mathcal{B}(\mathcal{L}^s, (\mathcal{L}^s)^*).$$

We replace $\mathcal{B}$ by $\mathcal{C}$ when considering the corresponding spaces of compact operators. Define the sequences $\mathbf{n} \in (\mathcal{L}^1)^*$ and $\mathbf{1} \in (\mathcal{L}^0)^*$ by

$$\mathbf{n}[m] = m \quad \text{and} \quad \mathbf{1}[m] = 1, \quad m \in \mathbb{N}, \tag{II.4}$$

respectively. Throughout the paper we frequently use the *pseudo-inverse* $A^\dagger$ of a self-adjoint operator A. For this concept we refer to Appendix A.

Proposition II.1. *Let $N \geq 0$ be any integer. As $\kappa \to 0$ with $\operatorname{Re}\kappa > 0$, the resolvent $R_0(\kappa)$ has the expansion:*

$$R_0(\kappa) = \sum_{j=0}^{N} \kappa^j G_{0,j} + \mathcal{O}(\kappa^{N+1}) \quad \text{in } \mathcal{B}^{N+2}, \tag{II.5}$$

with $G_{0,j} \in \mathcal{B}^{j+1}$ for j even, and $G_{0,j} \in \mathcal{B}^j$ for j odd, satisfying

$$\begin{aligned}
H_0 G_{0,0} &= G_{0,0} H_0 = I, \\
H_0 G_{0,1} &= G_{0,1} H_0 = 0, \\
H_0 G_{0,j} &= G_{0,j} H_0 = -G_{0,j-2} \quad \text{for } j \geq 2.
\end{aligned} \tag{II.6}$$

The coefficients $G_{0,j}$ have explicit kernels, and the first few are given by

$$G_{0,0}[n, m] = n \wedge m, \tag{II.7}$$

$$G_{0,1}[n, m] = -n \cdot m, \tag{II.8}$$

$$\begin{aligned}
G_{0,2}[n, m] &= -\tfrac{1}{6}(n \wedge m) \\
&\quad + \tfrac{1}{6}(n \wedge m)^3 + \tfrac{1}{2} n \cdot m \cdot (n \vee m),
\end{aligned} \tag{II.9}$$

$$G_{0,3}[n, m] = \tfrac{5}{24} n \cdot m - \tfrac{1}{6} n^3 \cdot m - \tfrac{1}{6} n \cdot m^3. \tag{II.10}$$

Proof. The expansion (II.5) with expressions (II.7)–(II.10) follows directly from (II.2), cf. Ito-Jensen[2] (Proposition 2.1). To see the identities in (II.6) it suffices to note that for any rapidly decreasing sequence $\Psi \colon \mathbb{N} \to \mathbb{C}$ we have

$$(H_0 + \kappa^2) R_0(\kappa) \Psi = R_0(\kappa)(H_0 + \kappa^2)\Psi = \Psi$$

for $\operatorname{Re}\kappa > 0$. The details of the computations are omitted. $\square$

We note that the sequence $\mathbf{n} \in (\mathcal{L}^1)^*$ is a *generalized eigenfunction* for H_0, and the coefficient $G_{0,1}$ is a *generalized projection* onto it:

$$H_0\mathbf{n} = 0, \quad G_{0,1} = -|\mathbf{n}\rangle\langle\mathbf{n}|.$$

On the other hand, the sequence $\mathbf{1} \in (\mathcal{L}^0)^*$, which with $\mathbf{n}$ forms a basis of the generalized eigenspace for the Laplacian on the whole line $\mathbb{Z}$, is not a generalized eigenfunction on $\mathbb{N}$. It does not appear in the above expansion coefficients, either.

III. THE PERTURBED LAPLACIAN

Now we consider the perturbed Laplacian $H = H_0 + V$ on $\mathbb{N}$, and state the main theorems of the paper. These theorems reveal a precise relation between the *generalized eigenspace* and the expansion coefficients of the resolvent at threshold.

The class of interactions considered here is from Ito-Jensen[2]. It is general enough to contain non-local interactions, but is formulated a little abstractly. We refer to Ito-Jensen[2] (Appendix B) for examples. We note that this class of interactions is closed under addition, see Ito-Jensen[2].

Recall the notation defined right before Proposition II.1.

Assumption III.1. Let $V \in \mathcal{B}(\mathcal{H})$ be self-adjoint, and assume that there exist an injective operator $v \in \mathcal{B}(\mathcal{K}, \mathcal{L}^\beta) \cap \mathcal{C}(\mathcal{K}, \mathcal{L}^1)$ with $\beta \geq 1$ and a self-adjoint unitary operator $U \in \mathcal{B}(\mathcal{K})$, both defined on some Hilbert space $\mathcal{K}$, such that

$$V = vUv^* \in \mathcal{B}((\mathcal{L}^\beta)^*, \mathcal{L}^\beta) \cap \mathcal{C}((\mathcal{L}^1)^*, \mathcal{L}^1).$$

Under Assumption III.1 we let

$$H = H_0 + V, \quad R(z) = (H - z)^{-1}.$$

The operator H is a bounded self-adjoint operator on $\mathcal{H}$ with $\sigma_{\mathrm{ess}}(H) = [0, 4]$. Using the Mourre method (see Boutet de Monvel-Shabani[5]) one can show that $\sigma_{\mathrm{sc}}(H) = \emptyset$. For local V other conditions for $\sigma_{\mathrm{sc}}(H) = \emptyset$ are given in Damanik-Killip[6].

Let us consider the solutions to the equation $H\Psi = 0$ in the largest space where it can be defined. Define the *(generalized) zero eigenspaces* by

$$\widetilde{\mathcal{E}} = \{\Psi \in (\mathcal{L}^\beta)^* \,|\, H\Psi = 0\}, \tag{III.1}$$

$$\mathcal{E} = \widetilde{\mathcal{E}} \cap (\mathbb{C}\mathbf{1} \oplus \mathcal{L}^{\beta-2}), \tag{III.2}$$

$$\mathsf{E} = \widetilde{\mathcal{E}} \cap \mathcal{L}^{\beta-2}. \tag{III.3}$$

These spaces will be analyzed in detail in Section V. Here we only quote some of the results given there: Under Assumption III.1 with $\beta \geq 1$ the generalized eigenfunctions have a specific asymptotics:

$$\widetilde{\mathcal{E}} \subset \mathbb{C}\mathbf{n} \oplus \mathbb{C}\mathbf{1} \oplus \mathcal{L}^{\beta-2}, \tag{III.4}$$

and their dimensions satisfy

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) + \dim(\mathcal{E}/\mathsf{E}) = 1, \quad 0 \leq \dim \mathsf{E} < \infty.$$

We introduce the same classification of the threshold as in Ito-Jensen[2] (Definition 1.6).

Definition III.2. The threshold $z = 0$ is said to be

1. a *regular point*, if $\mathcal{E} = \mathsf{E} = \{0\}$;
2. an *exceptional point of the first kind*, if $\mathcal{E} \supsetneq \mathsf{E} = \{0\}$;

3. an *exceptional point of the second kind*, if $\mathcal{E} = \mathsf{E} \supsetneq \{0\}$;
4. an *exceptional point of the third kind*, if $\mathcal{E} \supsetneq \mathsf{E} \supsetneq \{0\}$.

It would be more precise to call a function in $\widetilde{\mathcal{E}}$ a *generalized eigenfunction*, that in $\mathcal{E}$ a *resonance function*, and that in E an *eigenfunction*, but sometimes all of them are called simply *eigenfunctions*. In particular, we call $\Psi_c \in \mathcal{E}$ a *canonical resonance function* if it satisfies

$$\forall \Psi \in \mathsf{E} \ \ \langle \Psi, \Psi_c \rangle = 0, \quad \text{and} \quad \Psi_c - \mathbf{1} \in \mathcal{L}^{\beta-2}.$$

We remark that the latter asymptotics for $\Psi_c \in \mathcal{E}$ is equivalent to

$$\langle V\mathbf{n}, \Psi_c \rangle = -1.$$

We will prove this equivalence in Proposition V.1.

We now state the resolvent expansions in the four cases given in Definition III.2. We impose assumptions on the parameter β from Assumption III.1 in each of the four cases. For simplicity we state the results for integer values of β. The extension to general β is straightforward but leads to more complicated statements of the results and requires a different approach to the error estimates in the theorems below. Let us set

$$M_0 = U + v^* G_{0,0} v \colon \mathcal{K} \to \mathcal{K},$$

and denote its pseudo-inverse by $M_0^\dagger$, see Appendix A.

Theorem III.3. *Assume that the threshold* 0 *is a* regular *point, and that Assumption III.1 is fulfilled for some integer* $\beta \geq 2$. *Then*

$$R(\kappa) = \sum_{j=0}^{\beta-2} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-1}) \quad \textit{in } \mathcal{B}^{\beta-2} \tag{III.5}$$

with $G_j \in \mathcal{B}^{j+1}$ *for* j *even, and* $G_j \in \mathcal{B}^j$ *for* j *odd. The coefficients* G_j *can be computed explicitly. The first two coefficients can be expressed as*

$$G_0 = G_{0,0} - G_{0,0} v M_0^\dagger v^* G_{0,0}, \tag{III.6}$$
$$G_1 = -|\widetilde{\Psi}_c\rangle\langle\widetilde{\Psi}_c|, \tag{III.7}$$

where $\widetilde{\Psi}_c \in \widetilde{\mathcal{E}}$ *is a generalized eigenfunction with asymptotics*

$$m^{-1}\widetilde{\Psi}_c[m] \to 1 \quad \textit{as } m \to \infty.$$

Remark III.4. Under the assumption of Theorem III.3 the operator M_0 is actually invertible: $M_0^\dagger = M_0^{-1}$. The operators $I + G_{0,0}V$ and $I + VG_{0,0}$ are also invertible, and we have the expressions

$$I - G_{0,0} v M_0^\dagger v^* = (I + G_{0,0}V)^{-1}, \tag{III.8}$$
$$I - v M_0^\dagger v^* G_{0,0} = (I + VG_{0,0})^{-1}. \tag{III.9}$$

We will verify these right after the proof of Theorem III.3.

Theorem III.5. *Assume that the threshold* 0 *is an exceptional point of the* first kind, *and that Assumption III.1 is fulfilled for some integer* $\beta \geq 3$. *Then*

$$R(\kappa) = \sum_{j=-1}^{\beta-4} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-3}) \quad \textit{in } \mathcal{B}^{\beta-1} \tag{III.10}$$

with $G_j \in \mathcal{B}^{j+3}$ *for* j *even, and* $G_j \in \mathcal{B}^{j+2}$ *for* j *odd. The coefficients* G_j *can be computed explicitly. The first two coefficients can be expressed as*

$$G_{-1} = |\Psi_c\rangle\langle\Psi_c|, \tag{III.11}$$

$$\begin{aligned} G_0 = G_{0,0} &- \big(G_{0,0} - |\Psi_c\rangle\langle\mathbf{n}|\big) v M_0^\dagger v^* \big(G_{0,0} - |\mathbf{n}\rangle\langle\Psi_c|\big) \\ &- \big[\|\Psi_c - \mathbf{1}\|^2 + 2\,\mathrm{Re}\langle\mathbf{1}, \Psi_c - \mathbf{1}\rangle - \tfrac{1}{2}\big] |\Psi_c\rangle\langle\Psi_c| \\ &- |\Psi_c\rangle\langle\mathbf{n}| - |\mathbf{n}\rangle\langle\Psi_c|, \end{aligned} \tag{III.12}$$

where $\Psi_c \in \mathcal{E}$ *is the canonical resonance function.*

Theorem III.6. *Assume that the threshold* 0 *is an exceptional point of the* second kind, *and that Assumption III.1 is fulfilled for some integer* $\beta \geq 4$. *Then*

$$R(\kappa) = \sum_{j=-2}^{\beta-6} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-5}) \quad \text{in } \mathcal{B}^{\beta-2} \tag{III.13}$$

with $G_j \in \mathcal{B}^{j+3}$ *for* j *even, and* $G_j \in \mathcal{B}^{j+2}$ *for* j *odd. The coefficients* G_j *can be computed explicitly. The first four coefficients can be expressed as*

$$G_{-2} = P_0, \tag{III.14}$$

$$G_{-1} = 0, \tag{III.15}$$

$$G_0 = (I - P_0)\big(G_{0,0} - G_{0,0} v M_0^\dagger v^* G_{0,0}\big)(1 - P_0), \tag{III.16}$$

$$\begin{aligned} G_1 = (I - P_0)&\big(I - G_{0,0} v M_0^\dagger v^*\big) G_{0,1} \\ &\times \big(I - v M_0^\dagger v^* G_{0,0}\big)(I - P_0) \\ &- P_0 G_{0,0} v M_0^\dagger v^* G_{0,1} v M_0^\dagger v^* G_{0,0} P_0, \end{aligned} \tag{III.17}$$

where P_0 *is the projection onto* E.

Theorem III.7. *Assume that the threshold* 0 *is an exceptional point of the* third kind, *and that Assumption III.1 is fulfilled for some integer* $\beta \geq 4$. *Then*

$$R(\kappa) = \sum_{j=-2}^{\beta-6} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-5}) \quad \text{in } \mathcal{B}^{\beta-2} \tag{III.18}$$

with $G_j \in \mathcal{B}^{j+3}$ *for* j *even, and* $G_j \in \mathcal{B}^{j+2}$ *for* j *odd. The coefficients* G_j *can be computed explicitly. The first two coefficients can be expressed as*

$$G_{-2} = P_0,$$
$$G_{-1} = |\Psi_c\rangle\langle\Psi_c|,$$

where P_0 *is the projection onto* E, *and* $\Psi_c \in \mathcal{E}$ *is the canonical resonance function.*

By Theorems III.3–III.7, if $\beta \geq 4$, the resolvent $R(\kappa)$ always has an expansion of some order, and its threshold type can be determined by the coefficients G_{-2} and G_{-1}. We also state as a corollary certain identities satisfied by the coefficients.

Corollary III.8. *The coefficients* G_j *from Theorems III.3–III.7 satisfy*

$$\begin{aligned} HG_j &= G_j H = 0 \quad \text{for } j = -2, -1, \\ HG_0 &= G_0 H = I - P_0, \\ HG_j &= G_j H = -G_{j-2} \quad \text{for } j \geq 1, \end{aligned}$$

where P_0 *is the projection onto* E.

Proof. The assertion is verified by Theorems III.3–III.7 and the identities

$$(H + \kappa^2)R(\kappa)\Psi = R(\kappa)(H + \kappa^2)\Psi = \Psi$$

for any rapidly decreasing function $\Psi\colon \mathbb{N} \to \mathbb{C}$ and any $\kappa \sim 0$ with $\mathrm{Re}\,\kappa > 0$. □

We shall prove Theorems III.3–III.7 following the procedure given in Ito-Jensen[2]. The proofs will be given in Sections VII–X with preliminaries in the preceding sections.

IV. GENERAL BOUNDARY CONDITIONS

In this section we comment on discrete analogues of general boundary conditions at the origin of the half-line, such as the Neumann and the Robin conditions. In particular, we introduce specific potentials that allows us to deal with such a general boundary condition as a perturbation of the Dirichlet condition.

On the discrete half-line a boundary condition is realized simply by assigning a value to $x[0]$ for each function $x\colon \mathbb{N} \to \mathbb{C}$, as in (I.2). The natural realization of the Neumann boundary condition is to assign the difference there to be 0, i.e.,

$$x[1] - x[0] = 0 \quad \text{or} \quad x[0] = x[1].$$

Similarly, a more general Robin condition is realized by setting

$$ax[0] + b(x[0] - x[1]) = 0; \quad (a, b) \neq (0, 0).$$

Here we may take $a \neq -b$. Otherwise it reduces to the *shifted* Dirichlet condition $x[1] = 0$.

Let us remark that there is yet another realization of the Dirichlet boundary condition:

$$x[0] = -x[1], \tag{IV.1}$$

which models functions vanishing at $n = 1/2$. In other words, (IV.1) may be understood as arising from sampling a continuous function f at the points $n + 1/2$: $x[n] = f(n + 1/2)$. In such a model the Neumann condition is given by

$$x[1] - x[0] = 0,$$

and the Robin condition by

$$a(x[0] + x[1])/2 + b(x[1] - x[0]) = 0; \quad (a, b) \neq (0, 0).$$

In any case all the above boundary conditions are unified as

$$x[0] = \alpha x[1]; \quad \alpha \in \mathbb{R}.$$

Denote the corresponding Laplacian by H_α, i.e., for any sequence $x\colon \mathbb{N} \to \mathbb{C}$

$$(H_\alpha x)[n] = \begin{cases} (2-\alpha)x[1] - x[2] & \text{for } n = 1, \\ 2x[n] - x[n+1] - x[n-1] & \text{for } n \geq 2. \end{cases} \tag{IV.2}$$

We note that the operator H_α is in fact bounded and self-adjoint on $\mathcal{H} = \ell^2(\mathbb{N})$.

Let $e_1 = (1, 0, 0, \ldots)$ be the first canonical basis vector and define the potential

$$V_\alpha = -\alpha |e_1\rangle\langle e_1|. \tag{IV.3}$$

Then, comparing definitions (I.3) and (IV.2), we see that

$$H_\alpha = H_0 + V_\alpha. \tag{IV.4}$$

The potential V_α satisfies Assumption III.1 with $\mathcal{K} = \mathbb{C}$ and

$$v = \sqrt{|\alpha|}|e_1\rangle, \quad v^* = \sqrt{|\alpha|}\langle e_1|, \quad U = -\operatorname{sgn}\alpha. \tag{IV.5}$$

Actually V_α is a multiplication operator. We can directly compute

$$\widetilde{\mathcal{E}} = \mathbb{C}((1-\alpha)\mathbf{n} + \alpha\mathbf{1}), \quad \mathsf{E} = \{0\}.$$

Note that these eigenspaces can also be computed by applying the results of Section V to (IV.5). The above description of the eigenspaces implies the following:

Lemma IV.1. *The threshold* 0 *for the operator* H_α *is*

1. *a regular point if* $\alpha \neq 1$*;*
2. *an exceptional point of the first kind if* $\alpha = 1$*.*

We can construct the Fourier transform associated with H_α, and compute its expansion coefficients explicitly, which of course coincide with those computed from Theorems III.3–III.7 and Lemma IV.1. We remark that we may choose the Neumann Laplacian as the free operator, instead of the Dirichlet Laplacian, and formulate our main results for its perturbations. However, then the proofs get much more complicated, since its threshold 0 is an exceptional point of the first kind, which otherwise is regular.

V. GENERALIZED EIGENSPACES

In this section we write down the eigenspaces using subspaces of $\mathcal{K}$, and then derive some useful properties. In particular, we reveal the relation between invertibility of *intermediate operators* and threshold types. Compared with the full line discussed in Ito-Jensen[2], the half-line has a very clear correspondence between them, and the threshold structure is much simpler. This is because the free resolvent on the half-line does not have a singular term, and hence that of the perturbed resolvent comes only and directly from those intermediate operators.

To state the main results of this section let us introduce some notation. Let

$$M_0 = U + v^* G_{0,0} v, \quad M_1 = v^* G_{0,1} v = -|v^*\mathbf{n}\rangle\langle v^*\mathbf{n}|, \tag{V.1}$$

and $Q, S \in \mathcal{B}(\mathcal{K})$ be the orthogonal projections onto $\operatorname{Ker} M_0, \operatorname{Ker} M_1$, respectively. Then we set

$$m_0 = QM_1Q = -|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}|. \tag{V.2}$$

The operators M_0 and m_0 are, so to say, the *intermediate operators* in the terminology of Ito-Jensen[2] for the half-line case. They actually appear as expansion coefficients of certain operators in the later sections, but at least here we can define them independently of these expansions. They are well-defined for any $\beta \geq 1$ in Assumption III.1. In addition, we also define the operators $w \in \mathcal{B}((\mathcal{L}^\beta)^*, \mathcal{K})$ and $z \in \mathcal{B}(\mathcal{K}, \mathcal{L}^*)$ by

$$w = Uv^*, \quad z = \|v^*\mathbf{n}\|^{\dagger 2}\langle M_0 v^*\mathbf{n}, \cdot\,\rangle\mathbf{n} - G_{0,0}v, \tag{V.3}$$

where $a^\dagger$ denotes the pseudo-inverse of $a \in \mathbb{C}$, see (A.2).

Proposition V.1. *Suppose that* $\beta \geq 1$ *in Assumption III.1. Then the eigenspaces are expressed as*

$$\widetilde{\mathcal{E}} = z(\operatorname{Ker} SM_0) \oplus (\mathbb{C}\mathbf{n} \cap \operatorname{Ker} v^*), \tag{V.4}$$
$$\mathcal{E} = z(\operatorname{Ker} M_0), \tag{V.5}$$
$$\mathsf{E} = z(\operatorname{Ker} M_0 \cap \operatorname{Ker} M_1) = z(\operatorname{Ker} M_0 \cap \operatorname{Ker} m_0). \tag{V.6}$$

In particular, the generalized eigenfunctions have the special asymptotics (III.4)*, and, also, a function* $\Psi \in \mathcal{E}$ *has the asymptotics* $\Psi - \mathbf{1} \in \mathcal{L}^{\beta-2}$ *if and only if* $\langle V\mathbf{n}, \Psi\rangle = -1$*.*

Corollary V.2. *Suppose that $\beta \geq 1$ in Assumption III.1.*

1. *The threshold 0 is a regular point if and only if M_0 is invertible in $\mathcal{B}(\mathcal{K})$. In addition, if the threshold 0 is a regular point,*

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) = 1, \quad \dim(\mathcal{E}/\mathsf{E}) = \dim \mathsf{E} = 0.$$

2. *The threshold 0 is an exceptional point of the first kind if and only if M_0 is not invertible in $\mathcal{B}(\mathcal{K})$ and m_0 is invertible in $\mathcal{B}(Q\mathcal{K})$. In addition, if the threshold 0 is an exceptional point of the first kind,*

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) = 0, \quad \dim(\mathcal{E}/\mathsf{E}) = 1, \quad \dim \mathsf{E} = 0.$$

3. *The threshold 0 is an exceptional point of the second kind if and only if M_0 is not invertible in $\mathcal{B}(\mathcal{K})$ and $m_0 = 0$. In addition, if the threshold 0 is an exceptional point of the second kind,*

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) = 1, \quad \dim(\mathcal{E}/\mathsf{E}) = 0, \quad 1 \leq \dim \mathsf{E} < \infty.$$

4. *The threshold 0 is an exceptional point of the third kind if and only if M_0 and m_0 are not invertible in $\mathcal{B}(\mathcal{K})$ and $\mathcal{B}(Q\mathcal{K})$, respectively, and $m_0 \neq 0$. In addition, if the threshold 0 is an exceptional point of the third kind,*

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) = 0, \quad \dim(\mathcal{E}/\mathsf{E}) = 1, \quad 1 \leq \dim \mathsf{E} < \infty.$$

Corollary V.3. *Suppose that $\beta \geq 1$ in Assumption III.1, and that V is local. Then*

$$\dim \widetilde{\mathcal{E}} = 1, \quad \dim \mathsf{E} = 0, \tag{V.7}$$

i.e., the threshold 0 is either a regular point or an exceptional point of the first kind.

In the remainder of this section we prove Proposition V.1, and Corollaries V.2 and V.3, using a sequence of lemmas given below.

Lemma V.4. *For any $x \in \mathcal{L}^s$, $s \geq 1$, the sequence $G_{0,0}x \in \mathcal{L}^*$ is expressed as*

$$(G_{0,0}x)[n] = \langle \mathbf{n}, x \rangle - \sum_{m=n}^{\infty} (m-n)x[m] \quad \text{for } n \in \mathbb{N}. \tag{V.8}$$

In particular, $G_{0,0}x \in \mathcal{L}^{s-2}$ if and only if $\langle \mathbf{n}, x \rangle = 0$.

Proof. By (II.7) we can write

$$(G_{0,0}x)[n] = \sum_{m=1}^{n-1} mx[m] + \sum_{m=n}^{\infty} nx[m],$$

which immediately implies (V.8). Noting that

$$\sum_{n=1}^{\infty}(1+n^2)^{(s-2)/2}\left|\sum_{m=n}^{\infty}(m-n)x[m]\right| \leq C\|x\|_{1,s} < \infty,$$

we can deduce that the second term on the right-hand side of (V.8) belongs to $\mathcal{L}^{s-2}$. Then by the fact that $\mathbf{1} \notin \mathcal{L}^{s-2}$ for $s \geq 1$ we can verify the last assertion. □

Lemma V.5. *The compositions $H_0G_{0,0}$ and $G_{0,0}H_0$, defined on $\mathcal{L}^1$ and $\mathbb{C}\mathbf{n} \oplus \mathbb{C}\mathbf{1} \oplus \mathcal{L}^1$, respectively, are expressed as*

$$H_0G_{0,0} = I_{\mathcal{L}^1}, \quad G_{0,0}H_0 = \Pi,$$

where $\Pi\colon \mathbb{C}\mathbf{n} \oplus \mathbb{C}\mathbf{1} \oplus \mathcal{L}^1 \to \mathbb{C}\mathbf{1} \oplus \mathcal{L}^1$ is the projection.

Remark V.6. Lemmas V.4 and V.5 in particular imply that for any $s \geq 1$

$$\mathbb{C}\mathbf{1} \oplus \mathcal{L}^s \subset G_{0,0}(\mathcal{L}^s) \subset \mathbb{C}\mathbf{1} \oplus \mathcal{L}^{s-2}. \tag{V.9}$$

Proof. By direct computation employing the expression (V.8) we can verify that for any $x \in \mathcal{L}^1$

$$H_0 G_{0,0} x = G_{0,0} H_0 x = x.$$

We can also compute

$$H_0 \mathbf{n} = 0, \quad G_{0,0} H_0 \mathbf{1} = \mathbf{1}.$$

Then the assertion follows by the above identities. □

Lemma V.7. *For any* $\Phi \in \operatorname{Ker} SM_0$ *and* $\Psi \in \widetilde{\mathcal{E}}$

$$wz\Phi = \Phi, \quad zw\Psi \in \widetilde{\mathcal{E}}. \tag{V.10}$$

In addition,

$$z^{-1}(\widetilde{\mathcal{E}}) = \operatorname{Ker} SM_0, \qquad \widetilde{\mathcal{E}} \cap \operatorname{Ker} w = \mathbb{C}\mathbf{n} \cap \operatorname{Ker} v^*, \tag{V.11}$$
$$z^{-1}(\mathcal{E}) = \operatorname{Ker} M_0, \qquad \mathcal{E} \cap \operatorname{Ker} w = \{0\}, \tag{V.12}$$
$$z^{-1}(\mathsf{E}) = \operatorname{Ker} M_0 \cap \operatorname{Ker} M_1, \qquad \mathsf{E} \cap \operatorname{Ker} w = \{0\}. \tag{V.13}$$

Proof. Step 1. We prove the first assertion of (V.10). Let $\Phi \in \operatorname{Ker} SM_0$. Then, using $v^* G_{0,0} v = M_0 - U$, we can compute

$$\begin{aligned} wz\Phi &= Uv^*\Big[\|v^*\mathbf{n}\|^{2\dagger}\langle M_0 v^*\mathbf{n}, \Phi\rangle \mathbf{n} - G_{0,0} v\Phi\Big] \\ &= U(1-S)M_0\Phi - UM_0\Phi + \Phi \\ &= \Phi. \end{aligned}$$

Step 2. Before the second assertion of (V.10) we prove (V.11). We first note that by Lemma V.5 and $v^* G_{0,0} v = M_0 - U$ for any $\Phi \in \mathcal{K}$

$$\begin{aligned} Hz\Phi &= (H_0 + vUv^*)\Big[\|v^*\mathbf{n}\|^{2\dagger}\langle M_0 v^*\mathbf{n}, \Phi\rangle \mathbf{n} - G_{0,0} v\Phi\Big] \\ &= -v\Phi \\ &\quad + \|v^*\mathbf{n}\|^{2\dagger}\langle M_0 v^*\mathbf{n}, \Phi\rangle vUv^*\mathbf{n} - vU(M_0 - U)\Phi \\ &= -vUSM_0\Phi. \end{aligned} \tag{V.14}$$

Then, since vU is injective, it follows that $z\Phi \in \widetilde{\mathcal{E}}$ if and only if $\Phi \in \operatorname{Ker} SM_0$, which implies the first identity of (V.11). As for the second, we first note that for any $\Psi \in \widetilde{\mathcal{E}} \cap \operatorname{Ker} w$

$$H_0\Psi = 0, \quad v^*\Psi = 0.$$

Since the first identity $H_0\Psi = 0$ can be rephrased as $\Psi \in \mathbb{C}\mathbf{n}$, we obtain $\Psi \in \mathbb{C}\mathbf{n} \cap \operatorname{Ker} v^*$. The inverse inclusion is almost obvious, and hence the second identity of (V.11).

Step 3. Now we prove the second assertion of (V.10). Let $\Psi \in \widetilde{\mathcal{E}}$. Then by reusing (V.14) and noting $M_0 = U + v^* G_{0,0} v$ and Lemma V.5

$$\begin{aligned} Hzw\Psi &= -vUS(v^* + v^* G_{0,0} V)\Psi \\ &= -vUSv^* G_{0,0}(H_0 + V)\Psi \\ &= 0, \end{aligned}$$

which implies $zw\Psi \in \widetilde{\mathcal{E}}$.

Step 4. Let us prove (V.12). Let $\Phi \in \mathcal{K}$. By Lemma V.4 we can write

$$\begin{aligned} z\Phi[n] &= \|v^*\mathbf{n}\|^{2\dagger}\langle v^*\mathbf{n}, M_0\Phi\rangle\mathbf{n}[n] - \langle v^*\mathbf{n}, \Phi\rangle\mathbf{1}[n] \\ &\quad + \sum_{m=n}^{\infty}(m-n)(v\Phi)[m]. \end{aligned} \tag{V.15}$$

As in the proof of Lemma V.4, the last term in (V.15) belong to $\mathcal{L}^{\beta-2}$. This fact combined with the first identity of (V.11) implies that $z\Phi \in \mathcal{E}$ if and only if

$$\Phi \in \operatorname{Ker} SM_0, \quad \|v^*\mathbf{n}\|^{2\dagger}\langle v^*\mathbf{n}, M_0\Phi\rangle = 0.$$

Hence the first identity of (V.12) is obtained. As for the second one we can proceed as in Step 2, and it is almost obvious.

Step 5. The assertion (V.13) can be shown similarly to Step 4, and we omit the details. □

Proof of Proposition V.1. From (V.10) and the first identity of (V.11) we can deduce that the restrictions

$$z|_{\operatorname{Ker} SM_0}\colon \operatorname{Ker} SM_0 \to \widetilde{\mathcal{E}}, \quad w|_{\widetilde{\mathcal{E}}}\colon \widetilde{\mathcal{E}} \to \operatorname{Ker} SM_0$$

are injective and surjective, respectively. Hence, the asserted isomorphisms (V.4)–(V.6) are direct consequences of (V.11)–(V.13), respectively. We note that the last inequality of (V.6) is obvious by the definitions (V.1) and (V.2).

The asymptotics (III.4) follows immediately by (V.4), (V.3) and (V.9). Next, for any $\Psi \in \mathcal{E}$ we let $\Phi = w\Psi = Uv^*\Psi \in \operatorname{Ker} M_0$. Then, since $\Psi = z\Phi = -G_{0,0}v\Phi$, Lemma V.4 implies that $\Psi - \mathbf{1} \in \mathcal{L}^{\beta-2}$ if and only if $\langle \mathbf{n}, -v\Phi\rangle = 1$, which in turn is equivalent to $\langle V\mathbf{n}, \Psi\rangle = -1$. Hence we are done. □

Proof of Corollary V.2. We first claim that

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) \le 1, \quad \dim(\mathcal{E}/\mathsf{E}) \le 1, \quad \dim \mathsf{E} < \infty. \tag{V.16}$$

The first and second inequalities of (V.16) are obvious by (III.4), (III.2) and (III.3). For the last inequality of (V.16) we note that $Uv^*G_{0,0}v \in \mathcal{C}(\mathcal{K})$. Then

$$\begin{aligned} \dim \mathsf{E} \le \dim \mathcal{E} &= \dim \operatorname{Ker} M_0 \\ &= \dim \operatorname{Ker}(1 + Uv^*G_{0,0}v) < \infty. \end{aligned}$$

Hence the claim follows.

Now we prove the assertions 1–4 of the corollary. We note that the former parts of 1–4 are obvious by Proposition V.1, and hence we may discuss only the latter parts.

1. Let the threshold 0 be a regular point. Then by definition we have

$$\dim \mathcal{E} = \dim \mathsf{E} = 0.$$

If $v^*\mathbf{n} = 0$, then, since $S = I_{\mathcal{K}}$, we have by (V.4) that $\widetilde{\mathcal{E}} = \mathbb{C}\mathbf{n}$. Otherwise, noting that M_0 is invertible, we have by (V.4) that $\widetilde{\mathcal{E}} = \mathbb{C}zM^{-1}v^*\mathbf{n}$. In either cases we can conclude that

$$\dim \widetilde{\mathcal{E}} = 1.$$

2. Let the threshold 0 be an exceptional point of the first kind. Then by definition and claim (V.16)

$$\dim \mathcal{E} = 1, \quad \dim \mathsf{E} = 0.$$

Let us show that $\widetilde{\mathcal{E}} = \mathcal{E}$. Since $Q\mathcal{K}$ is nontrivial and $m_0 = -|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}|$ is invertible there, it follows that

$$Qv^*\mathbf{n} \neq 0. \tag{V.17}$$

Now it suffices to show that $\operatorname{Ker} SM_0 \subset \operatorname{Ker} M_0$. Let $\Phi \in \operatorname{Ker} SM_0$. Since S is the orthogonal projections onto the kernel of M_1 given by (V.1), there exists $c \in \mathbb{C}$ such that

$$M_0\Phi = cv^*\mathbf{n}.$$

Apply Q to both sides above, then by (V.17) it follows that $c = 0$. Hence $\Phi \in \operatorname{Ker} M_0$, and the latter assertion is verified.

3. Let the threshold 0 be an exceptional point of the second kind. Then by definition and claim (V.16)

$$\dim(\mathcal{E}/\mathsf{E}) = 0, \quad 1 \leq \dim \mathsf{E} < \infty.$$

If $v^*\mathbf{n} = 0$, then $S = I_{\mathcal{K}}$, and hence by (V.4)

$$\widetilde{\mathcal{E}} = z(\operatorname{Ker} M_0) \oplus \mathbb{C}\mathbf{n} = \mathcal{E} \oplus \mathbb{C}\mathbf{n}.$$

Otherwise, since $m_0 = -|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}| = 0$, we have

$$0 \neq v^*\mathbf{n} \in (\operatorname{Ker} M_0)^{\perp} = \operatorname{Ran} M_0,$$

and hence we can find $\Phi \in \mathcal{K} \setminus \{0\}$ such that $M_0\Phi = v^*\mathbf{n}$. Such Φ is unique up to $\operatorname{Ker} M_0$, and then by (V.4)

$$\widetilde{\mathcal{E}} = z(\operatorname{Ker} M_0 \oplus \mathbb{C}\Phi) = \mathcal{E} \oplus \mathbb{C}z\Phi.$$

In either cases we obtain

$$\dim(\widetilde{\mathcal{E}}/\mathcal{E}) = 1.$$

4. Let the threshold 0 be an exceptional point of the third kind. Then by definition and claim (V.16)

$$\dim(\mathcal{E}/\mathsf{E}) = 1, \quad 1 \leq \dim \mathsf{E} < \infty.$$

Now it suffices to show that $\widetilde{\mathcal{E}} = \mathcal{E}$, but this can be proved exactly the same manner as in the proof of the assertion 2 above. Hence we are done. □

Proof of Corollary V.3. It suffces to show that $\mathsf{E} = \{0\}$. Let $\Psi \in \mathsf{E}$. Then it follows by Lemma V.7 that $\Psi = zw\Psi$. This equation can be rephrased as

$$\Psi[n] = \sum_{m=n}^{\infty} (m-n)V[m]\Psi[m] \tag{V.18}$$

by Lemma V.4 and the asymptotics of Ψ as $n \to \infty$. Since $V \in \mathcal{L}^\beta$, we can choose large $n_0 \geq 0$ such that

$$\sum_{n=n_0}^{\infty} n|V[n]| \leq \tfrac{1}{2}. \tag{V.19}$$

By (V.18) and (V.19) we obtain

$$\bigl|\Psi[n]\bigr| \leq \tfrac{1}{2} \sup_{m \geq n_0} \bigl|\Psi[m]\bigr| \text{ for } n \geq n_0,$$

or

$$\Psi[n] = 0 \text{ for } n \geq n_0.$$

Since the equation $H\Psi = 0$ is a difference equation, the above initial condition at infinity yields $\Psi = 0$, and hence $\mathsf{E} = \{0\}$. Hence we are done. □

VI. THE FIRST STEP IN RESOLVENT EXPANSION

This section gives a short preliminary computation for the proofs of Theorems III.3–III.7 given in the following sections. These computations are common to all the proofs.

Define the operator $M(\kappa) \in \mathcal{B}(\mathcal{K})$ for $\operatorname{Re}\kappa > 0$ by

$$M(\kappa) = U + v^* R_0(\kappa) v. \tag{VI.1}$$

Fix $\kappa_0 > 0$ such that $z = -\kappa^2$ belongs to the resolvent set of H for any $\operatorname{Re}\kappa \in (0, \kappa_0)$. This is possible due to the decay assumptions on V.

Lemma VI.1. *Let the operator $M(\kappa)$ be defined as above.*

1. *Let Assumption III.1 hold for some integer $\beta \geq 2$. Then*

$$M(\kappa) = \sum_{j=0}^{\beta-2} \kappa^j M_j + \mathcal{O}(\kappa^{\beta-1}) \quad \text{in } \mathcal{B}(\mathcal{K}) \tag{VI.2}$$

with $M_j \in \mathcal{B}(\mathcal{K})$ given by

$$M_0 = U + v^* G_{0,0} v, \quad M_j = v^* G_{0,j} v \text{ for } j \geq 1. \tag{VI.3}$$

2. *Let Assumption III.1 hold with $\beta \geq 1$. For any $0 < \operatorname{Re}\kappa < \kappa_0$ the operator $M(\kappa)$ is invertible in $\mathcal{B}(\mathcal{K})$, and*

$$M(\kappa)^{-1} = U - Uv^* R(\kappa) v U.$$

Moreover,

$$R(\kappa) = R_0(\kappa) - R_0(\kappa) v M(\kappa)^{-1} v^* R_0(\kappa). \tag{VI.4}$$

Proof. 1. This result follows from Assumption III.1 and Proposition II.1.

2. The assertion is verified by direct computations, see Ito-Jensen[2] (Proposition 1.13). □

Note that the operators M_0 and M_1 coincide with those defined in Section V.

By Lemma VI.1.1 the operator $M(\kappa)$ has an expansion, and by Lemma VI.1.2 and Proposition II.1 an expansion of $R(\kappa)$ is reduced to that of the inverse $M(\kappa)^{-1}$. If the leading operator $M_0 \in \mathcal{B}(\mathcal{K})$ is invertible, or by Proposition V.1, if the threshold 0 is a regular point, we can employ the Neumann series to compute the expansion of $M(\kappa)^{-1}$. Otherwise, we shall employ an inversion formula introduced in Jensen-Nenciu[3] in a way similar to Ito-Jensen[2]. We note that we are also going to use the pseudo-inverse several times. For reference we present the inversion formula and the pseudo-inverse in Appendix A.

VII. REGULAR THRESHOLD

In this section we prove Theorem III.3. In this case the leading operator M_0 in the expansion (VI.2) is invertible by Corollary V.2. Hence the inversion formula in Appendix A is not needed.

Proof of Theorem III.3. By the assumption and Corollary V.2 it follows that M_0 is invertible in $\mathcal{B}(\mathcal{K})$. Hence we can use the Neumann series to invert (VI.2). Let us write it as

$$M(\kappa)^{-1} = \sum_{j=0}^{\beta-2} \kappa^j A_j + \mathcal{O}(\kappa^{\beta-1}), \quad A_j \in \mathcal{B}(\mathcal{K}). \tag{VII.1}$$

The coefficients A_j are written explicitly in terms of the M_j. The first two terms are

$$A_0 = M_0^{-1}, \quad A_1 = -M_0^{-1}M_1M_0^{-1}. \tag{VII.2}$$

We insert the expansions (II.5) with $N = \beta - 2$ and (VII.1) into (VI.4), and then obtain the expansion

$$R(\kappa) = \sum_{j=0}^{\beta-2} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-1});$$
$$G_j = G_{0,j} - \sum_{\substack{j_1\ge0, j_2\ge0, j_3\ge0\\ j_1+j_2+j_3=j}} G_{0,j_1} v A_{j_2} v^* G_{0,j_3}.$$

This result and (VII.2) in particular leads to the expressions

$$\begin{aligned} G_0 &= G_{0,0} - G_{0,0}vM_0^{-1}v^*G_{0,0}, \\ G_1 &= G_{0,1} - G_{0,1}vM_0^{-1}v^*G_{0,0} \\ &\quad + G_{0,0}vM_0^{-1}M_1M_0^{-1}v^*G_{0,0} - G_{0,0}vM_0^{-1}v^*G_{0,1} \\ &= (I - G_{0,0}vM_0^{-1}v^*)G_{0,1}(I - vM_0^{-1}v^*G_{0,0}). \end{aligned}$$

The expression (III.6) is obtained. The expression (III.7) follows by noting

$$(I - G_{0,0}vM_0^{-1}v^*)\mathrm{n} = \widetilde{\Psi}_c,$$

which can be verified with ease by (V.4). □

Verification of (III.9). The first identity in (III.9) follows by

$$\begin{aligned} &(I+G_{0,0}V)(I - G_{0,0}vM_0^{-1}v^*) \\ &\quad = I - G_{0,0}vM_0^{-1}v^* + G_{0,0}V - G_{0,0}VG_{0,0}vM_0^{-1}v^* \\ &\quad = I - G_{0,0}vU(U + v^*G_{0,0}v)M_0^{-1}v^* + G_{0,0}V \\ &\quad = I, \end{aligned}$$

$$\begin{aligned} &(I - G_{0,0}vM_0^{-1}v^*)(I + G_{0,0}V) \\ &\quad = I - G_{0,0}vM_0^{-1}v^* + G_{0,0}V - G_{0,0}vM_0^{-1}v^*G_{0,0}V \\ &\quad = I - G_{0,0}vM_0^{-1}(U + v^*G_{0,0}v)Uv^* + G_{0,0}V \\ &\quad = I. \end{aligned}$$

The second identity is verified analogously. □

VIII. EXCEPTIONAL THRESHOLD OF THE FIRST KIND

In this section we prove Theorem III.5. In this case the leading operator $M_0 \in \mathcal{B}(\mathcal{K})$ in (VI.2) is not invertible, and we need the inversion formula given in Appendix A to invert the expansion (VI.2).

Proof of Theorem III.5. By the assumption and Corollary V.2 the leading operator M_0 from (VI.2) is not invertible in $\mathcal{B}(\mathcal{K})$, and we are going to apply Proposition A.2. Let us write the expansion (VI.2) as

$$M(\kappa) = \sum_{j=0}^{\beta-2} \kappa^j M_j + \mathcal{O}(\kappa^{\beta-1}) = M_0 + \kappa\widetilde{M}_1(\kappa). \tag{VIII.1}$$

Let Q be the orthogonal projection onto Ker M_0, cf. Section V, and define

$$m(\kappa) = \sum_{j=0}^{\infty} (-1)^j \kappa^j Q \widetilde{M}_1(\kappa) \big[(M_0^\dagger + Q) \widetilde{M}_1(\kappa) \big]^j Q. \tag{VIII.2}$$

Then by Proposition A.2 we have

$$\begin{aligned} M(\kappa)^{-1} &= (M(\kappa) + Q)^{-1} \\ &\quad + \frac{1}{\kappa} (M(\kappa) + Q)^{-1} m(\kappa)^\dagger (M(\kappa) + Q)^{-1}. \end{aligned} \tag{VIII.3}$$

Note that by using (VIII.1) we can rewrite (VIII.2) in the form

$$m(\kappa) = \sum_{j=0}^{\beta-3} \kappa^j m_j + \mathcal{O}(\kappa^{\beta-2}); \quad m_j \in \mathcal{B}(Q\mathcal{K}). \tag{VIII.4}$$

We have the following expressions for the first four coefficients:

$$m_0 = QM_1Q, \tag{VIII.5}$$

$$m_1 = QM_2Q - QM_1(M_0^\dagger + Q)M_1Q, \tag{VIII.6}$$

$$\begin{aligned} m_2 &= QM_3Q - QM_1(M_0^\dagger + Q)M_2Q \\ &\quad - QM_2(M_0^\dagger + Q)M_1Q \\ &\quad + QM_1(M_0^\dagger + Q)M_1(M_0^\dagger + Q)M_1Q, \end{aligned} \tag{VIII.7}$$

$$\begin{aligned} m_3 &= QM_4Q - QM_1(M_0^\dagger + Q)M_3Q \\ &\quad - QM_2(M_0^\dagger + Q)M_2Q - QM_3(M_0^\dagger + Q)M_1Q \\ &\quad + QM_1(M_0^\dagger + Q)M_1(M_0^\dagger + Q)M_2Q \\ &\quad + QM_1(M_0^\dagger + Q)M_2(M_0^\dagger + Q)M_1Q \\ &\quad + QM_2(M_0^\dagger + Q)M_1(M_0^\dagger + Q)M_1Q \\ &\quad - QM_1(M_0^\dagger + Q)M_1(M_0^\dagger + Q)M_1(M_0^\dagger + Q)M_1Q. \end{aligned} \tag{VIII.8}$$

Then by the assumption and Corollary V.2 the coefficient $m_0 = QM_1Q$ is invertible in $\mathcal{B}(Q\mathcal{K})$. Thus the Neumann series provides the expansion of the inverse $m(\kappa)^\dagger$. Let us write it as

$$\begin{gathered} m(\kappa)^\dagger = \sum_{j=0}^{\beta-3} \kappa^j A_j + \mathcal{O}(\kappa^{\beta-2}), \\ A_0 = m_0^\dagger, \quad A_j \in \mathcal{B}(Q\mathcal{K}). \end{gathered} \tag{VIII.9}$$

The Neumann series also provide an expansion of $(M(\kappa) + Q)^{-1}$, which we write as

$$(M(\kappa) + Q)^{-1} = \sum_{j=0}^{\beta-2} \kappa^j B_j + \mathcal{O}(\kappa^{\beta-1}), \tag{VIII.10}$$

where $B_j \in \mathcal{B}(\mathcal{K})$. The first three coefficients can be written as follows:

$$\begin{aligned} B_0 &= M_0^\dagger + Q, \\ B_1 &= -(M_0^\dagger + Q)M_1(M_0^\dagger + Q), \\ B_2 &= -(M_0^\dagger + Q)M_2(M_0^\dagger + Q) \\ &\quad + (M_0^\dagger + Q)M_1(M_0^\dagger + Q)M_1(M_0^\dagger + Q). \end{aligned}$$

Now we insert the expansions (VIII.9) and (VIII.10) into the formula (VIII.3), and then

$$\begin{aligned} M(\kappa)^{-1} &= \sum_{j=-1}^{\beta-4} \kappa^j C_j + \mathcal{O}(\kappa^{\beta-3}), \\ C_j &= B_j + \sum_{\substack{j_1\ge 0, j_2\ge 0, j_3\ge 0\\ j_1+j_2+j_3=j+1}} B_{j_1} A_{j_2} B_{j_3}, \end{aligned} \tag{VIII.11}$$

with $B_{-1} = 0$. Next we insert the expansions (II.5) with $N = \beta - 3$ and (VIII.11) into the formula (VI.4). Then we obtain the expansion

$$\begin{aligned} R(\kappa) &= \sum_{j=-1}^{\beta-4} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-3}), \\ G_j &= G_{0,j} - \sum_{\substack{j_1\ge 0, j_2\ge -1, j_3\ge 0\\ j_1+j_2+j_3=j}} G_{0,j_1} v C_{j_2} v^* G_{0,j_3}, \end{aligned}$$

with $G_{0,-1} = 0$. This verifies (III.10).

Next we compute G_{-1}. By the above expressions we can write

$$G_{-1} = -G_{0,0} v C_{-1} v^* G_{0,0} = -G_{0,0} v m_0^\dagger v^* G_{0,0},$$

and by (II.8)

$$m_0 = Q M_1 Q = -|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}|. \tag{VIII.12}$$

The expression (VIII.12) implies that m_0 is at most of rank 1, but by the assumption and Corollary V.2 it is also invertible in $\mathcal{B}(Q\mathcal{K})$. Hence it follows that

$$Qv^*\mathbf{n} \neq 0, \quad \dim \operatorname{Ker} M_0 = \dim Q\mathcal{K} = 1.$$

Then we can write

$$m_0^\dagger = -|\Phi_c\rangle\langle\Phi_c|; \tag{VIII.13}$$

$$\Phi_c = -\|Qv^*\mathbf{n}\|^{-2} Qv^*\mathbf{n} \in Q\mathcal{K} = \operatorname{Ker} M_0, \tag{VIII.14}$$

such that

$$G_{-1} = |\Psi_c\rangle\langle\Psi_c|; \quad \Psi_c = -G_{0,0} v \Phi_c \in \mathcal{E}.$$

Let us to show that the above resonance function Ψ_c is canonical. We have

$$\langle V\mathbf{n}, \Psi_c\rangle = -\langle v^*\mathbf{n}, U(M_0 - U)\Phi_c\rangle = \langle v^*\mathbf{n}, \Phi_c\rangle = -1,$$

and hence we obtain (III.11).

Finally we prove (III.12). We first express G_0 by A_* and B_*, and then insert expressions for them:

$$\begin{aligned} G_0 &= G_{0,0} - G_{0,0} v C_{-1} v^* G_{0,1} - G_{0,1} v C_{-1} v^* G_{0,0} \\ &\quad - G_{0,0} v C_0 v^* G_{0,0} \\ &= G_{0,0} - G_{0,0} v A_0 v^* G_{0,1} - G_{0,1} v A_0 v^* G_{0,0} \\ &\quad - G_{0,0} v \big(B_0 + B_0 A_0 B_1 + B_1 A_0 B_0 \\ &\qquad + B_0 A_1 B_0\big) v^* G_{0,0} \\ &= G_{0,0} - G_{0,0} v m_0^\dagger v^* G_{0,1} - G_{0,1} v m_0^\dagger v^* G_{0,0} \\ &\quad - G_{0,0} v \Big(M_0^\dagger + Q - m_0^\dagger M_1 (M_0^\dagger + Q) \\ &\qquad - (M_0^\dagger + Q) M_1 m_0^\dagger - m_0^\dagger m_1 m_0^\dagger\Big) v^* G_{0,0}. \end{aligned}$$

We expand the terms in big parentheses and unfold m_1, noting $m_0 m_0^\dagger = m_0^\dagger m_0 = Q$:

$$\begin{aligned}
G_0 &= G_{0,0} - G_{0,0} v m_0^\dagger v^* G_{0,1} - G_{0,1} v m_0^\dagger v^* G_{0,0} \\
&\quad - G_{0,0} v \Big(M_0^\dagger - m_0^\dagger M_1 M_0^\dagger - M_0^\dagger M_1 m_0^\dagger \\
&\qquad - m_0^\dagger M_2 m_0^\dagger + m_0^\dagger M_1 M_0^\dagger M_1 m_0^\dagger \Big) v^* G_{0,0} \\
&= G_{0,0} + G_{0,0} v m_0^\dagger M_2 m_0^\dagger v^* G_{0,0} - G_{0,0} v m_0^\dagger v^* G_{0,1} \\
&\quad - G_{0,1} v m_0^\dagger v^* G_{0,0} \\
&\quad - G_{0,0} v (I - m_0^\dagger M_1) M_0^\dagger (I - M_1 m_0^\dagger) v^* G_{0,0}.
\end{aligned}$$

Now we use (VIII.14) and the expressions $M_j = v^* G_{0,j} v$, $j \geq 1$, and $G_{0,1} = -|\mathbf{n}\rangle\langle\mathbf{n}|$:

$$\begin{aligned}
G_0 &= G_{0,0} + |\Psi_c\rangle\langle v\Phi_c, G_{0,2} v\Phi_c\rangle\langle\Psi_c| - |\Psi_c\rangle\langle\mathbf{n}| - |\mathbf{n}\rangle\langle\Psi_c| \\
&\quad - \big(G_{0,0} - |\Psi_c\rangle\langle\mathbf{n}|\big) v M_0^\dagger v^* \big(G_{0,0} - |\mathbf{n}\rangle\langle\Psi_c|\big).
\end{aligned}$$

Hence it remains to compute the coefficient of the second term in the last expression. We have by $\Phi_c = Uv\Psi$

$$\langle v\Phi_c, G_{0,2} v\Phi_c\rangle = \langle V\Psi_c, G_{0,2} V\Psi_c\rangle = \langle H_0\Psi_c, G_{0,2} H_0\Psi_c\rangle.$$

Here we remark that we cannot directly use $G_{0,2} H_0 = -G_{0,0}$, since (II.6) holds as an extension from rapidly decaying functions, while Ψ_c is not decaying. However, it suffices to subtract the leading asymptotics as follows.

$$\begin{aligned}
&\langle v\Phi_c, G_{0,2} v\Phi_c\rangle \\
&\quad = \big\langle H_0(\Psi_c - \mathbf{1}), G_{0,2} H_0\Psi_c\big\rangle + (G_{0,2} H_0 \Psi_c)[1] \\
&\quad = -\big\langle (\Psi_c - \mathbf{1}), G_{0,0} H_0 \Psi_c\big\rangle \\
&\qquad + \big(G_{0,2} H_0(\Psi_c - \mathbf{1})\big)[1] + (G_{0,2} H_0 \mathbf{1})[1] \\
&\quad = -\big\langle (\Psi_c - \mathbf{1}), G_{0,0} H_0 (\Psi_c - \mathbf{1})\big\rangle \\
&\qquad - \overline{(G_{0,0}(\Psi_c - \mathbf{1}))[1]} \\
&\qquad - \big(G_{0,0}(\Psi_c - \mathbf{1})\big)[1] + (G_{0,2} H_0 \mathbf{1})[1] \\
&\quad = -\|\Psi_c - \mathbf{1}\|^2 - 2\,\mathrm{Re}(G_{0,0}(\Psi_c - \mathbf{1}))[1] \\
&\qquad + (G_{0,2} H_0 \mathbf{1})[1].
\end{aligned}$$

The last two terms are computed by using the explicit expressions (II.7) and (II.9). Then we obtain (III.12). □

IX. EXCEPTIONAL THRESHOLD OF THE SECOND KIND

Here we prove Theorem III.6. For the first part of the proof we can almost repeat the argument of the previous section, but the second part is rather non-trivial. In fact, we need the following lemma.

Lemma IX.1. *Let $x_\nu \in \mathcal{L}^4$, $\nu = 1, 2$. Assume that*

$$\langle \mathbf{n}, x_\nu\rangle = 0, \quad \nu = 1, 2. \tag{IX.1}$$

Then one has that $G_{0,0} x_\nu \in \mathcal{L}^2$, $\nu = 1, 2$, and that

$$\langle x_1, G_{0,2} x_2\rangle = -\langle G_{0,0} x_1, G_{0,0} x_2\rangle. \tag{IX.2}$$

Proof. We extend the sequences $x_\nu \in \mathcal{L}^4$, $\nu = 1, 2$, antisymmetrically to the whole line $\mathbb{Z}$ by letting

$$\widetilde{x}_\nu[n] = \operatorname{sgn}[n] x_\nu[|n|], \quad n \in \mathbb{Z}.$$

Noting that the kernels $G_{0,0}[n,m]$ and $G_{0,2}[n,m]$ have the expressions

$$\begin{aligned} G_{0,0}[n,m] &= -\tfrac{1}{2}\big(|n-m| - (n+m)\big), \\ G_{0,2}[n,m] &= \tfrac{1}{12}\big(|n-m| - |n-m|^3 \\ &\qquad - (n+m) + (n+m)^3\big), \end{aligned}$$

we also define operators $\widetilde{G}_{0,0}$ and $\widetilde{G}_{0,2}$ mapping antisymmetric functions on $\mathbb{Z}$ to themselves by the integral kernels

$$\begin{aligned} \widetilde{G}_{0,0}[n,m] &= -\tfrac{1}{2}|n-m|, \\ \widetilde{G}_{0,2}[n,m] &= \tfrac{1}{12}\big(|n-m| - |n-m|^3\big), \end{aligned} \tag{IX.3}$$

respectively. Then it is easy to check that for $\nu = 1, 2$, $j = 0, 2$ and $n \geq 1$

$$(G_{0,j} x_\nu)[n] = (\widetilde{G}_{0,j}\widetilde{x}_\nu)[n] = -(\widetilde{G}_{0,j}\widetilde{x}_\nu)[-n]. \tag{IX.4}$$

On the other hand, the kernels (IX.3) are the same as the convolution kernels in Ito-Jensen[2] (equation (2.5)), and hence under assumption (IX.1) Ito-Jensen[2] (Lemma 4.16) applies. It follows that $\widetilde{G}_{0,0}\widetilde{x}_\nu \in \ell^{1,2}(\mathbb{Z})$ and that

$$\langle \widetilde{x}_1, \widetilde{G}_{0,2}\widetilde{x}_2\rangle = -\langle \widetilde{G}_{0,0}\widetilde{x}_1, \widetilde{G}_{0,0}\widetilde{x}_2\rangle. \tag{IX.5}$$

Then by (IX.4) and (IX.5) the assertion follows. □

Proof of Theorem III.6. By the assumption and Corollary V.2 the leading operator M_0 from (VI.2) is not invertible in $\mathcal{B}(\mathcal{K})$. Write the expansion (VI.2) in the same form as (VIII.1), let Q be the orthogonal projection onto Ker M_0, and define $m(\kappa)$ by the same formula as (VIII.2). Then by Proposition A.2 we have the same formula as (VIII.3). Again, $m(\kappa)$ defined by (VIII.2) has the same expansion (VIII.4) with the same expressions (VIII.5)–(VIII.8) for its coefficients, but this time we actually have

$$m_0 = 0, \quad m_1 = QM_2Q, \quad m_2 = 0. \tag{IX.6}$$

In fact, by the assumption we have

$$\begin{aligned} m_0 = QM_1Q = -|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}| = 0, \\ \text{or} \quad Qv^*\mathbf{n} = 0, \end{aligned} \tag{IX.7}$$

and hence (IX.6) follows by (VI.3), (II.8), (IX.7) and (VIII.5)–(VIII.8). Now we note that then the operator m_1 has to be invertible in $\mathcal{B}(Q\mathcal{K})$. Otherwise, we can apply Proposition A.2 once more, but this leads to a singularity of order κ^{-j}, $j \geq 3$, in the expansion of $R(\kappa)$, which contradicts the self-adjointness of H. Hence the Neumann series provides an expansion of $m(\kappa)^\dagger$ of the form

$$m(\kappa)^\dagger = \sum_{j=-1}^{\beta-5} \kappa^j A_j + \mathcal{O}(\kappa^{\beta-4}), \quad A_j \in \mathcal{B}(Q\mathcal{K}), \tag{IX.8}$$

with, e.g.

$$\begin{aligned} A_{-1} = m_1^\dagger, \quad A_0 = -m_1^\dagger m_2 m_1^\dagger, \\ A_1 = -m_1^\dagger m_3 m_1^\dagger + m_1^\dagger m_2 m_1^\dagger m_2 m_1^\dagger. \end{aligned}$$

These are actually simplified by (IX.6) as

$$A_{-1} = m_1^\dagger, \quad A_0 = 0, \quad A_1 = -m_1^\dagger m_3 m_1^\dagger. \tag{IX.9}$$

The Neumann series also provides an expansion of $(M(\kappa) + Q)^{-1}$ in the same form as (VIII.10) with the same coefficients given there. Now we insert the expansions (IX.8) and (VIII.10) into the formula (VIII.3), and then

$$\begin{aligned} M(\kappa)^{-1} &= \sum_{j=-2}^{\beta-6} \kappa^j C_j + \mathcal{O}(\kappa^{\beta-5}); \\ C_j &= B_j + \sum_{\substack{j_1\ge 0, j_2\ge -1, j_3\ge 0\\ j_1+j_2+j_3=j+1}} B_{j_1} A_{j_2} B_{j_3} \end{aligned} \tag{IX.10}$$

with $B_{-2} = B_{-1} = 0$. We then insert the expansions (II.5) with $N = \beta - 4$ and (IX.10) into the formula (VI.4). Finally we obtain the expansion

$$\begin{aligned} R(\kappa) &= \sum_{j=-2}^{\beta-6} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-5}); \\ G_j &= G_{0,j} - \sum_{\substack{j_1\ge 0, j_2\ge -2, j_3\ge 0\\ j_1+j_2+j_3=j}} G_{0,j_1} v C_{j_2} v^* G_{0,j_3} \end{aligned}$$

with $G_{0,-2} = G_{0,-1} = 0$.

Next we compute the coefficients. We can use the above expressions of the coefficients to write

$$\begin{aligned} G_{-2} &= -G_{0,0} v C_{-2} v^* G_{0,0} \\ &= -G_{0,0} v m_1^\dagger v^* G_{0,0} \\ &= z(Qv^* G_{0,2} v Q)^\dagger z^*. \end{aligned} \tag{IX.11}$$

By this expression we can see that

$$\operatorname{Ran} G_{-2} = (\operatorname{Ker} G_{-2})^\perp \subset \mathcal{E} = \mathsf{E}.$$

In addition, by Proposition V.1 for any $\Psi \in \mathsf{E}$ we can write $\Psi = z\Phi = -G_{0,0} v\Phi$ for some $\Phi \in Q\mathcal{K}$, so that by Lemma IX.1

$$\begin{aligned} \langle \Psi, G_{-2}\Psi\rangle &= -\langle G_{0,0} v\Phi, G_{0,0} v (Qv^* G_{0,2} vQ)^\dagger z^*\Psi\rangle \\ &= \|\Psi\|^2_{\mathcal{H}}. \end{aligned}$$

Since G_{-2} is obviously self-adjoint on E, this implies that G_{-2} coincides with the orthogonal projection P_0 onto E, as asserted in (III.14).

As for G_{-1}, we can first write

$$\begin{aligned} G_{-1} = &-G_{0,0} v C_{-1} v^* G_{0,0} \\ &- G_{0,0} v C_{-2} v^* G_{0,1} - G_{0,1} v C_{-2} v^* G_{0,0}. \end{aligned}$$

If we make use of the vanishing in (IX.6), (IX.7) and (IX.9), we can easily verify (III.15) from this expression. We omit the details.

Next, we compute G_1. Let us write, implementing $B_0 A_* = A_* B_0 = A_*$,

$$\begin{aligned} G_0 &= G_{0,0} - G_{0,0} v C_0 v^* G_{0,0} \\ &\quad - G_{0,0} v C_{-1} v^* G_{0,1} - G_{0,1} v C_{-1} v^* G_{0,0} \\ &\quad - G_{0,0} v C_{-2} v^* G_{0,2} - G_{0,1} v C_{-2} v^* G_{0,1} \\ &\quad - G_{0,2} v C_{-2} v^* G_{0,0} \\ &= G_{0,0} - G_{0,0} v \big(B_0 + A_1 + A_0 B_1 + B_1 A_0 \\ &\qquad + B_1 A_{-1} B_1 + A_{-1} B_2 + B_2 A_{-1} \big) v^* G_{0,0} \\ &\quad - G_{0,0} v \big(A_0 + A_{-1} B_1 + B_1 A_{-1} \big) v^* G_1 \\ &\quad - G_{0,1} v \big(A_0 + A_{-1} B_1 + B_1 A_{-1} \big) v^* G_{0,0} \\ &\quad - G_{0,0} v A_{-1} v^* G_{0,2} - G_{0,1} v A_{-1} v^* G_{0,1} \\ &\quad - G_{0,2} v A_{-1} v^* G_{0,0}. \end{aligned}$$

Let us now use some vanishing relations coming from (IX.6), (IX.7), and (IX.9):

$$\begin{aligned} G_0 &= G_{0,0} - G_{0,0} v \big(B_0 + A_1 + B_1 A_{-1} B_1 \\ &\qquad + A_{-1} B_2 + B_2 A_{-1} \big) v^* G_{0,0} \\ &\quad - G_{0,0} v A_{-1} B_1 v^* G_{0,1} - G_{0,1} v B_1 A_{-1} v^* G_{0,0} \\ &\quad - G_{0,0} v A_{-1} v^* G_{0,2} - G_{0,2} v A_{-1} v^* G_{0,0}, \end{aligned}$$

and then insert expressions for A_* and B_*, noting the kernels of operators and implementing (IX.6) and (IX.7). We omit some computations, obtaining

$$\begin{aligned} G_0 &= G_{0,0} - G_{0,0} v \Big(M_0^\dagger + Q - m_1^\dagger m_3 m_1^\dagger \\ &\qquad - m_1^\dagger M_2 (M_0^\dagger + Q) - (M_0^\dagger + Q) M_2 m_1^\dagger \Big) v^* G_{0,0} \\ &\quad - G_{0,0} v m_1^\dagger v^* G_{0,2} - G_{0,2} v m_1^\dagger v^* G_{0,0}. \end{aligned}$$

Next we unfold m_3. We use the expressions $m_3 = Q M_4 Q - Q M_2 M_0^\dagger M_2 Q - m_1 m_1$ and $Q M_2 Q = m_1$ which hold under (IX.7), and then

$$\begin{aligned} G_0 &= G_{0,0} - G_{0,0} v (I - m_1^\dagger M_2) M_0^\dagger (I - M_2 m_1^\dagger) v^* G_{0,0} \\ &\quad - G_{0,0} v \big(Q + m_1^\dagger m_1 m_1 m_1^\dagger \\ &\qquad - m_1^\dagger m_1 - m_1 m_1^\dagger \big) v^* G_{0,0} \\ &\quad - G_{0,0} v m_1^\dagger v^* G_{0,2} - G_{0,2} v m_1^\dagger v^* G_{0,0} \\ &\quad + G_{0,0} v m_1^\dagger M_4 m_1^\dagger v^* G_{0,0}. \end{aligned}$$

Now we note that by (IX.11) we have

$$m_1^\dagger = -U v^* P_0 v U \tag{IX.12}$$

and this operator is bijective as $Q\mathcal{K} \to Q\mathcal{K}$. Hence we have

$$\begin{aligned} G_0 &= G_{0,0} - (G_{0,0} + P_0 V G_{0,2}) v M_0^\dagger v^* (G_{0,0} + G_{0,2} V P_0) \\ &\quad + P_0 V G_{0,2} + G_{0,2} V P_0 + P_0 V G_{0,4} V P_0 \end{aligned}$$

Furthermore, we make use of the identities $V P_0 = -H_0 P_0$, $P_0 V = -P_0 H_0$ and $H_0 G_{0,j} = G_{0,j} H_0 = G_{0,j-2}$ for $j \geq 2$:

$$\begin{aligned} G_0 &= G_{0,0} - (G_{0,0} - P_0 G_{0,0}) v M_0^\dagger v^* (G_{0,0} - G_{0,0} P_0) \\ &\quad - P_0 G_{0,0} - G_{0,0} P_0 + P_0 G_{0,0} P_0 \\ &= (I - P_0) \big[G_{0,0} \\ &\qquad - G_{0,0} v (U + v^* G_{0,0} v)^\dagger v^* G_{0,0} \big] (1 - P_0). \end{aligned}$$

This verifies (III.16).

The computation of G_1 in this case is very long, and we do not present all the detail in this paper. We only describe some of important steps. First we can write it, using only A_* and B_*,

$$\begin{aligned}
G_1 = G_{0,1}& \\
&- G_{0,0}vA_{-1}v^*G_{0,3} - G_{0,1}vA_{-1}v^*G_{0,2} \\
&- G_{0,2}vA_{-1}v^*G_{0,1} - G_{0,3}vA_{-1}v^*G_{0,0} \\
&- G_{0,0}v\big(A_{-1}B_1 + B_1A_{-1} + A_0\big)v^*G_{0,2} \\
&- G_{0,1}v\big(A_{-1}B_1 + B_1A_{-1} + A_0\big)v^*G_{0,1} \\
&- G_{0,2}v\big(A_{-1}B_1 + B_1A_{-1} + A_0\big)v^*G_{0,0} \\
&- G_{0,0}v\big(B_0 + A_{-1}B_2 + B_1A_{-1}B_1 \\
&\quad + B_2A_{-1}\big)v^*G_{0,1} \\
&- G_{0,1}v\big(B_0 + A_{-1}B_2 + B_1A_{-1}B_1 \\
&\quad + B_2A_{-1}\big)v^*G_{0,0} \\
&- G_{0,0}v\big(B_1 + A_{-1}B_3 + B_1A_{-1}B_2 \\
&\quad + B_2A_{-1}B_1 + B_3A_{-1} + A_0B_2 + B_1A_0B_1 \\
&\quad + B_2A_0 + A_1B_1 + B_1A_1 + A_2\big)v^*G_{0,0}.
\end{aligned}$$

Then we insert the expressions of A_* and B_*. If we implement some of vanishing relations coming from (IX.6), (IX.7), and (IX.9), we arrive at

$$\begin{aligned}
G_1 = G_{0,1} &- G_{0,0}vm_1^\dagger v^*G_{0,3} - G_{0,3}vm_1^\dagger v^*G_{0,0} \\
&- G_{0,0}v\big(M_0^\dagger - m_1^\dagger M_2M_0^\dagger\big)v^*G_{0,1} \\
&- G_{0,1}v\big(M_0^\dagger - M_0^\dagger M_2m_1^\dagger\big)v^*G_{0,0} \\
&- G_{0,0}v\Big[-M_0^\dagger M_1M_0^\dagger \\
&\quad + m_1^\dagger(-M_3M_0^\dagger + M_2M_0^\dagger M_1M_0^\dagger) \\
&\quad + (-M_0^\dagger M_3 + M_0^\dagger M_1M_0^\dagger M_2)m_1^\dagger \\
&\quad - m_1^\dagger m_4m_1^\dagger\Big]v^*G_{0,0}.
\end{aligned}$$

If we insert (IX.12) and $m_4 = QM_5Q - QM_2JM_3Q - QM_3JM_2Q$, which holds especially in this case due to the vanishing relations noted above, we come to

$$\begin{aligned}
G_1 = G_{0,1} &+ G_{0,0}VP_0VG_{0,3} + G_{0,3}VP_0VG_{0,0} \\
&- G_{0,0}\big(vM_0^\dagger v^* + VP_0VG_{0,2}vM_0^\dagger v^*\big)G_{0,1} \\
&- G_{0,1}\big(vM_0^\dagger v^* + vM_0^\dagger v^*G_{0,2}VP_0V\big)G_{0,0} \\
&- G_{0,0}\Big[-vM_0^\dagger v^*G_{0,1}vM_0^\dagger v^* + VP_0VG_{0,3}vM_0^\dagger v^* \\
&\quad - VP_0VG_{0,2}vM_0^\dagger v^*G_{0,1}vM_0^\dagger v^* \\
&\quad + vM_0^\dagger v^*G_{0,3}VP_0V \\
&\quad - vM_0^\dagger v^*G_{0,1}vM_0^\dagger v^*G_{0,2}VP_0V \\
&\quad - VP_0VG_{0,5}VP_0V \\
&\quad + VP_0VG_{0,2}vM_0^\dagger v^*G_{0,3}VP_0V \\
&\quad + VP_0VG_{0,3}vM_0^\dagger v^*G_{0,2}VP_0V\Big]G_{0,0}.
\end{aligned}$$

Finally we use $VP_0 = -H_0P_0$, $P_0V = -P_0H_0$ and (II.6), and then the expression (III.17) is obtained. Hence we are done. $\square$

X. EXCEPTIONAL THRESHOLD OF THE THIRD KIND

Finally we prove Theorem III.7. Compared with the proof of Theorem III.6, this case needs one more application of the inversion formula, or Proposition A.2, and the formulas get much more complicated.

Proof of Theorem III.7. Let us repeat arguments of the previous section to some extent. We write the expansion (VI.2) in the same form as (VIII.1), let Q be the orthogonal projection onto $\operatorname{Ker} M_0$, and define $m(\kappa)$ by the same formula as (VIII.2). Then by Proposition A.2 we have the same formula as (VIII.3), again. The operator $m(\kappa)$ defined by (VIII.2) has the same expansion as (VIII.4) with (VIII.5)–(VIII.8), but without (IX.6) or (IX.7) by the assumption and Corollary V.2. Now we apply the inversion formula, Proposition A.2, to the operator $m(\kappa)$. Write the expansion (VIII.4) in the form

$$m(\kappa) = m_0 + \kappa\widetilde{m}_1(\kappa). \tag{X.1}$$

The leading operator m_0 is non-zero and not invertible in $\mathcal{B}(Q\mathcal{K})$ by the assumption and Corollary V.2. Let T be the orthogonal projection onto $\operatorname{Ker} m_0 \subset Q\mathcal{K}$, and set

$$q(\kappa) = \sum_{j=0}^{\infty}(-1)^j\kappa^j T\widetilde{m}_1(\kappa)\big[(m_0^\dagger + T)\widetilde{m}_1(\kappa)\big]^j T. \tag{X.2}$$

Then we have by Proposition A.2 that

$$\begin{aligned} m(\kappa)^\dagger &= (m(\kappa)+T)^\dagger \\ &\quad + \frac{1}{\kappa}(m(\kappa)+T)^\dagger q(\kappa)^\dagger (m(\kappa)+T)^\dagger. \end{aligned} \tag{X.3}$$

Using (VIII.4) and (X.1), let us write (X.2) in the form

$$q(\kappa) = \sum_{j=0}^{\beta-4}\kappa^j q_j + \mathcal{O}(\kappa^{\beta-3}); \quad q_j \in \mathcal{B}(T\mathcal{K}).$$

The first and the second coefficients are given as

$$q_0 = Tm_1T, \quad q_1 = Tm_2T - Tm_1(m_0^\dagger + T)m_1T. \tag{X.4}$$

Here we note that the leading operator q_0 has to be invertible in $\mathcal{B}(T\mathcal{K})$. Otherwise, applying Proposition A.2 once again, we can show that $R(\kappa)$ has a singularity of order κ^{-j}, $j \geq 3$ in its expansion. This contradicts the self-adjointness of H. Hence we can use the Neumann series to write $q(\kappa)^\dagger$, and obtain

$$q(\kappa)^\dagger = \sum_{j=0}^{\beta-4}\kappa^j A_j + \mathcal{O}(\kappa^{\beta-3}), \quad A_j \in \mathcal{B}(T\mathcal{K}), \tag{X.5}$$

where

$$A_0 = q_0^\dagger, \quad A_1 = -q_0^\dagger q_1 q_0^\dagger.$$

We also write $(m(\kappa)+T)^\dagger$ employing the Neumann series as

$$(m(\kappa)+T)^\dagger = \sum_{j=0}^{\beta-3}\kappa^j C_j + \mathcal{O}(\kappa^{\beta-2}) \tag{X.6}$$

with $C_j \in \mathcal{B}(Q\mathcal{K})$ and

$$C_0 = m_0^\dagger + T, \quad C_1 = -(m_0^\dagger + T)m_1(m_0^\dagger + T).$$

We first insert the expansions (X.5) and (X.6) into (X.3):

$$m(\kappa)^\dagger = \sum_{j=-1}^{\beta-5} \kappa^j D_j + \mathcal{O}(\kappa^{\beta-4}), \tag{X.7}$$
$$D_j = C_j + \sum_{\substack{j_1\ge 0, j_2\ge 0, j_3\ge 0\\ j_1+j_2+j_3=j+1}} C_{j_1} A_{j_2} C_{j_3},$$

with $C_{-1} = 0$. Next, noting that we have an expansion of $(M(\kappa)+Q)^{-1}$ in the same form as (VIII.10), we insert the expansions (X.7) and (VIII.10) into (VIII.3):

$$M(\kappa)^{-1} = \sum_{j=-2}^{\beta-6} \kappa^j E_j + \mathcal{O}(\kappa^{\beta-5}), \tag{X.8}$$
$$E_j = B_j + \sum_{\substack{j_1\ge 0, j_2\ge -1, j_3\ge 0\\ j_1+j_2+j_3=j+1}} B_{j_1} D_{j_2} B_{j_3},$$

with $B_{-2} = B_{-1} = 0$. We finally inserting the expansions (II.5) with $N = \beta - 4$ and (X.8) into (VI.4), and then obtain the expansion

$$R(\kappa) = \sum_{j=-2}^{\beta-6} \kappa^j G_j + \mathcal{O}(\kappa^{\beta-5}),$$
$$G_j = G_{0,j} - \sum_{\substack{j_1\ge 0, j_2\ge -2, j_3\ge 0\\ j_1+j_2+j_3=j}} G_{0,j_1} v E_{j_2} v^* G_{0,j_3},$$

with $G_{0,-2} = G_{0,-1} = 0$.

Next we compute the first two coefficients. Let us start with G_{-2}. Unfolding the above expressions, we can see with ease that

$$\begin{aligned} G_{-2} &= -G_{0,0} v E_{-2} v^* G_{0,0} \\ &= -G_{0,0} v \big(TM_2T - TM_1(M_0^\dagger + T)M_1T\big)^\dagger v^* G_{0,0}. \end{aligned}$$

Since

$$m_0 = QM_1Q = -|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}|, \tag{X.9}$$

it follows that

$$Tv^*\mathbf{n} = TQv^*\mathbf{n} = 0. \tag{X.10}$$

Hence we have

$$G_{-2} = -G_{0,0} v (Tv^* G_{0,2} vT)^\dagger v^* G_{0,0},$$

and we can verify the identity $G_{-2} = P_0$ in exactly the same manner as in the proof of Theorem III.6.

As for G_{-1}, it requires a slightly longer computations, and we proceed step by step. We can first write, concerning A_*, B_*, C_*, D_*, E_* only,

$$\begin{aligned}
G_{-1} &= -G_{0,0}vE_{-1}v^*G_{0,0} - G_{0,0}vE_{-2}v^*G_{0,1} \\
&\quad - G_{0,1}vE_{-2}v^*G_{0,0} \\
&= -G_{0,0}v\Big(B_0\big(C_0 + C_0A_1C_0 \\
&\qquad + C_0A_0C_1 + C_1A_0C_0\big)B_0 \\
&\qquad + B_0C_0A_0C_0B_1 + B_1C_0A_0C_0B_0\Big)v^*G_{0,0} \\
&\quad - G_{0,0}vB_0C_0A_0C_0B_0v^*G_{0,1} \\
&\quad - G_{0,1}vB_0C_0A_0C_0B_0v^*G_{0,0}.
\end{aligned}$$

Next, we implement the identities $B_0C_* = C_*B_0 = C_*$ and $C_0A_* = A_*C_0 = A_*$, insert expressions of A_*, B_*, C_*, and then use (X.10):

$$\begin{aligned}
G_{-1} &= -G_{0,0}v\Big(C_0 + A_1 + A_0C_1 \\
&\qquad + C_1A_0 + A_0B_1 + B_1A_0\Big)v^*G_{0,0} \\
&\quad - G_{0,0}vA_0v^*G_{0,1} - G_{0,1}vA_0v^*G_{0,0} \\
&= -G_{0,0}v\Big(m_0^\dagger + T - q_0^\dagger q_1 q_0^\dagger - q_0^\dagger m_1(m_0^\dagger + T) \\
&\qquad - (m_0^\dagger + T)m_1q_0^\dagger \\
&\qquad - q_0^\dagger M_1(M_0^\dagger + Q) - (M_0^\dagger + Q)M_1q_0^\dagger\Big)v^*G_{0,0} \\
&\quad - G_{0,0}vq_0^\dagger v^*G_{0,1} - G_{0,1}vq_0^\dagger v^*G_{0,0}. \\
&= -G_{0,0}v\Big(m_0^\dagger + T - q_0^\dagger q_1 q_0^\dagger - q_0^\dagger m_1(m_0^\dagger + T) \\
&\qquad - (m_0^\dagger + T)m_1q_0^\dagger\Big)v^*G_{0,0}.
\end{aligned}$$

We further unfold q_1 and m_1 and use (X.10):

$$\begin{aligned}
G_{-1} &= -G_{0,0}v\Big(m_0^\dagger + T + q_0^\dagger M_2(m_0^\dagger + T)M_2q_0^\dagger \\
&\qquad - q_0^\dagger M_2(m_0^\dagger + T) - (m_0^\dagger + T)M_2q_0^\dagger\Big)v^*G_{0,0} \\
&= -G_{0,0}v(I - q_0^\dagger M_2)m_0^\dagger(I - M_2q_0^\dagger)v^*G_{0,0} \\
&\quad - G_{0,0}v(I - q_0^\dagger M_2)T(I - M_2q_0^\dagger)v^*G_{0,0}.
\end{aligned}$$

Since $TM_2T = Tm_1T = q_0T$ by (X.10), the last term can actually be removed:

$$G_{-1} = -G_{0,0}v(I - q_0^\dagger M_2)m_0^\dagger(I - M_2q_0^\dagger)v^*G_{0,0}.$$

Finally by (X.9) we can write

$$m_0^\dagger = -\|Qv^*\mathbf{n}\|^{-4}|Qv^*\mathbf{n}\rangle\langle Qv^*\mathbf{n}|,$$

and hence we obtain

$$\begin{aligned}
G_{-1} &= |\Psi_c\rangle\langle\Psi_c|, \\
\Psi_c &= \|Qv^*\mathbf{n}\|^{-2}G_{0,0}v(I - q_0^\dagger v^*G_{0,2}v)Qv^*\mathbf{n} \in \mathcal{E}.
\end{aligned}$$

Let us verify that the above Ψ_c is in fact the canonical resonance function. For any $\Psi \in \mathsf{E}$ set $\Phi = w\Psi \in T\mathcal{K}$. As in the proof of Theorem III.6 we can verify that

$$\begin{aligned}\langle \Psi, \Psi_c\rangle &= -\|Qv^*\mathbf{n}\|^{-2}\\ &\quad\times \big\langle G_{0,0}vT\Phi, G_{0,0}v(I - q_0^\dagger v^* G_{0,2}v)Qv^*\mathbf{n}\big\rangle\\ &= 0.\end{aligned}$$

We can also prove that

$$\begin{aligned}\langle V\mathbf{n}, \Psi_c\rangle &= \|Qv^*\mathbf{n}\|^{-2}\\ &\quad\times \big\langle V\mathbf{n}, G_{0,0}v(I - q_0^\dagger v^* G_{0,2}v)Qv^*\mathbf{n}\big\rangle\\ &= \|Qv^*\mathbf{n}\|^{-2}\\ &\quad\times \big\langle Uv^*\mathbf{n}, (M_0 - U)(I - q_0^\dagger v^* G_{0,2}v)Qv^*\mathbf{n}\big\rangle\\ &= -\|Qv^*\mathbf{n}\|^{-2}\big\langle v^*\mathbf{n}, (I - q_0^\dagger v^* G_{0,2}v)Qv^*\mathbf{n}\big\rangle\\ &= -1.\end{aligned}$$

This concludes the proof. □

Appendix A: Inversion formula

In this appendix we present an inversion formula needed in the proof of the main results of the paper. The formula is quoted from Ito-Jensen[2] (Section 3.1), which in turn was adapted from Jensen-Nenciu[3] (Corollary 2.2).

Let us argue in a general context.

Assumption A.1. Let $\mathcal{K}$ be a Hilbert space and $A(\kappa)$ a family of bounded operators on $\mathcal{K}$ with $\kappa \in D \subset \mathbb{C} \setminus \{0\}$. Suppose that

1. The set $D \subset \mathbb{C}\setminus\{0\}$ is invariant under complex conjugation and accumulates at $0 \in \mathbb{C}$.
2. For each $\kappa \in D$ the operator $A(\kappa)$ satisfies $A(\kappa)^* = A(\overline{\kappa})$ and has a bounded inverse $A(\kappa)^{-1} \in \mathcal{B}(\mathcal{K})$.
3. As $\kappa \to 0$ in D, the operator $A(\kappa)$ has an expansion in the uniform topology of the operators at $\mathcal{K}$:
$$A(\kappa) = A_0 + \kappa\widetilde{A}_1(\kappa); \quad \widetilde{A}_1(\kappa) = \mathcal{O}(1). \tag{A.1}$$
4. The spectrum of A_0 does not accumulate at $0 \in \mathbb{C}$ as a set.

If the leading operator A_0 is invertible in $\mathcal{B}(\mathcal{K})$, the Neumann series provides an inversion formula for the expansion of $A(\kappa)^{-1}$:

$$A(\kappa)^{-1} = \sum_{j=0}^{\infty}(-1)^j\kappa^j A_0^{-1}\big[\widetilde{A}_1(\kappa)A_0^{-1}\big]^j.$$

The inversion formula given below is useful when A_0 is not invertible in $\mathcal{B}(\mathcal{K})$.

We define the *pseudo-inverse* $a^\dagger$ for a complex number $a \in \mathbb{C}$ by

$$a^\dagger = \begin{cases} 0 & \text{if } a = 0,\\ a^{-1} & \text{if } a \neq 0.\end{cases} \tag{A.2}$$

Let $\mathcal{K}' \subset \mathcal{K}$ be a closed subspace. We always identify $\mathcal{B}(\mathcal{K}')$ with its embedding in $\mathcal{B}(\mathcal{K})$ in the standard way. For an operator $A \in \mathcal{B}(\mathcal{K}') \subset \mathcal{B}(\mathcal{K})$ we say that A is *invertible in* $\mathcal{B}(\mathcal{K}')$ if there exists an operator $A^\dagger \in \mathcal{B}(\mathcal{K}')$ such that $A^\dagger A = AA^\dagger = I_{\mathcal{K}'}$, which we identify with the orthogonal projection onto $\mathcal{K}' \subset \mathcal{K}$ as noted. For a general self-adjoint operator A on $\mathcal{K}$ we abuse the notation $A^\dagger$ also to denote the operator defined by the usual operational calculus for the function (A.2). The operator $A^\dagger$ for a self-adjoint operator A belongs to $B(\mathcal{K})$ if and only if the spectrum of A does not accumulate at 0 as a set, and in such a case the above two $A^\dagger$ coincide. In either case we call $A^\dagger$ the *pseudo-inverse* of A. The reader should note that we always use the notation A^* for the adjoint and the notation $A^\dagger$ for the pseudo-inverse.

Proposition A.2. *Suppose Assumption A.1. Let Q be the orthogonal projection onto* $\operatorname{Ker} A_0$, *and define the operator $a(\kappa) \in \mathcal{B}(Q\mathcal{K})$ by*

$$\begin{aligned} a(\kappa) &= \tfrac{1}{\kappa}\{I_{Q\mathcal{K}} - Q(A(\kappa)+Q)^{-1}Q\} \\ &= \sum_{j=0}^{\infty}(-1)^j\kappa^j Q\widetilde{A}_1(\kappa)\big[(A_0^\dagger + Q)\widetilde{A}_1(\kappa)\big]^j Q. \end{aligned} \tag{A.3}$$

Then $a(\kappa)$ is bounded in $\mathcal{B}(Q\mathcal{K})$ as $\kappa \to 0$ in D. Moreover, for each $\kappa \in D$ sufficiently close to 0 the operator $a(\kappa)$ is invertible in $\mathcal{B}(Q\mathcal{K})$, and

$$\begin{aligned} A(\kappa)^{-1} &= (A(\kappa)+Q)^{-1} \\ &\quad + \frac{1}{\kappa}(A(\kappa)+Q)^{-1}a(\kappa)^\dagger(A(\kappa)+Q)^{-1}. \end{aligned} \tag{A.4}$$

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