

# Spectral and scattering properties at thresholds for the Laplacian in a half-space with a periodic boundary condition

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## Abstract

For the scattering system given by the Laplacian in a half-space with a periodic boundary condition, we derive resolvent expansions at embedded thresholds, we prove the continuity of the scattering matrix, and we establish new formulas for the wave operators.

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## 1 Introduction

We present in this paper new results for the Laplacian in a half-space subject to a periodic boundary condition, as introduced and described by R. L. Frank and R. G. Shterenberg in [12, 13, 14]. We derive resolvent expansions at embedded thresholds (which occur in an infinite number after a Floquet decomposition), we prove the continuity of the scattering matrix at thresholds, and we establish new representation formulas for the wave operators. These results belong to the intersection of two active research topics in spectral and scattering theory. On one hand, resolvent expansions at thresholds (which have a long history, but which have been more systematically developed since the seminal paper of A. Jensen and G. Nenciu [20], see also [11, 17, 21, 28]). On the second hand, representation formulas for the wave operators and their application to the proof of index theorems in scattering theory (see [5, 16, 23, 24, 26, 27, 29] and references therein). These results also furnish a new contribution to the very short list of papers devoted to the subtle, and still poorly understood, topic of spectral and scattering theory at embedded thresholds (to our knowledge only the references [6, 7, 8, 10, 15, 28] deal specifically with this issue).

Before giving a more precise description of our results, we recall the definition and some of the properties (established in [12, 13, 14]) of the model we consider. The model consists in a scattering system  $\{H^0, H^V\}$ , where  $H^V$  (the perturbed operator) is the Laplacian on the half-space  $\mathbb{R} \times \mathbb{R}_+$  subject to a boundary condition on  $\mathbb{R} \times \{0\}$  given in terms of a  $2\pi$ -periodic function  $V : \mathbb{R} \rightarrow \mathbb{R}$ , and where  $H^0$  (the unperturbed operator) is the Neumann Laplacian on  $\mathbb{R} \times \mathbb{R}_+$ . An application of a Bloch-Floquet-Gelfand transform in the periodic variable shows that the pair  $\{H^0, H^V\}$  is unitarily equivalent to a family

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of self-adjoint operators  $\{H_k^0, H_k^V\}_{k \in [-1/2, 1/2]}$  acting in the Hilbert space  $L^2((-\pi, \pi) \times \mathbb{R}_+)$ . The operators  $H_k^0$  have purely absolutely continuous spectrum, whereas the operators  $H_k^V$  have no singular continuous spectrum but can have discrete spectrum (with only possible accumulation point at  $+\infty$ ). Under suitable conditions on  $V$ , it is known that the wave operators  $W_{k,\pm} := W_{\pm}(H_k^0, H_k^V)$  exist and are complete, and that the full wave operators  $W_{\pm} := W_{\pm}(H^0, H^V)$  exist, but may be not complete. The states belonging to the cokernel of  $W_{\pm}$  are interpreted as *surface states*; that is, states which propagate along the boundary  $\mathbb{R} \times \{0\}$ .

The completeness of the wave operators  $W_{k,\pm}$  and the intertwining property imply that the scattering operator  $S_k := W_{k,+}^* W_{k,-}$  is unitary and decomposable in the spectral representation of  $H_k^0$ . However, since the spectral multiplicity of  $H_k^0$  is piecewise constant with a jump at each point of the threshold set

$$\tau_k := \{\lambda_{k,n} := (n+k)^2 \mid n \in \mathbb{Z}\},$$

the scattering matrix  $S_k(\lambda)$  can only be defined for  $\lambda \notin \tau_k$ . Therefore, the continuity of  $S_k(\lambda)$  in  $\lambda$  can only be proved in a suitable sense. By introducing channels corresponding to the transverse modes on the interval  $(-\pi, \pi)$ , we show that  $S_k(\lambda)$  is continuous at the thresholds if the channels we consider are already open, and that  $S_k(\lambda)$  has a limit from the right at the thresholds if a channel precisely opens at these thresholds (see Theorem 4.1 for a more precise statement). Also, we give explicit formulas for  $S_k(\lambda)$  at thresholds. To our knowledge, this type of results has never been obtained before except in [28], in the context of quantum waveguides. Our proof of the continuity properties relies on a stationary representation for  $S_k(\lambda)$  and on resolvent expansions for  $H_k^V$  at embedded thresholds. The resolvent expansions are proved in Proposition 3.3 under the single assumption that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$ . Information about the localization of the possible eigenvalues of  $H_k^V$  is also given in Section 3.

Section 5 is devoted to the derivation of representation formulas for the wave operators  $W_{k,\pm}$ . The main result of the section are formulas

$$W_{k,-} - 1 = (1 \otimes R(A_+))(S_k - 1) + \text{Rem} \quad \text{and} \quad W_{k,+} - 1 = (1 - 1 \otimes R(A_+))(S_k^* - 1) + \text{Rem},$$

where  $R$  is the function given by  $R(x) := \frac{1}{2}(1 + \tanh(\pi x) + i \cosh(\pi x)^{-1})$ ,  $A_+$  is the generator of dilations in  $\mathbb{R}_+$ , and  $\text{Rem}$  is a remainder term which is small in a suitable sense (see Lemma 5.7). This type of formulas has recently been derived for various scattering systems and is at the root of a topological approach of Levinson's theorem, see [24] for more explanations on this approach. Finally, collecting the previous identities for all values  $k$ , we obtain in Theorem 5.8 similar representations formulas for the full wave operators  $W_{\pm}(H^0, H^V)$ .

The content of this paper stops here and corresponds to the analytical part of a larger research project. As a motivation for further studies, we briefly sketch the sequel of the project here. Under some stronger assumption on  $V$ , for instance if  $V$  is a trigonometric polynomial, we expect the remainder term  $\text{Rem}$  to be a compact operator. In such a case, by using appropriate techniques of K-theory and  $C^*$ -algebras, one could relate the orthogonal projection on the bound states of  $H_k^V$  to the scattering operator  $S_k$  plus some correction terms due to threshold effects. We refer for example to [26, Sec. 3] for a presentation of the algebraic techniques in a much simpler setting. Then, using direct integrals to collect the results for all values of  $k$ , one would automatically obtain a relation between the orthogonal projection on the surface states of  $H^V$  and operators involved in the scattering process. This relation would be of a topological nature, it would have an interpretation in the general context of bulk-edge correspondence, and it would be completely new for such a continuous model. For discrete models, related results have been obtained in [9] for ergodic operators and in [29] for deterministic operators.

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## 2 Laplacian in a half-space

In this section, we recall the basic properties of the model we consider, which consists in a Laplacian on the half-space  $\mathbb{R} \times \mathbb{R}_+$ , with  $\mathbb{R}_+ := (0, \infty)$ , subject to a periodic boundary condition on  $\mathbb{R} \times \{0\}$ . Most of the material we present here is borrowed from the papers [12, 13] to which we refer for further information.

We choose a  $2\pi$ -periodic function  $V \in L^\infty(\mathbb{R}; \mathbb{R})$ , and for each non-empty open set  $\Omega \subset \mathbb{R}^n$ ,  $n \in \mathbb{N}^*$ , and each  $m \in \mathbb{N}$ , we denote by  $\mathcal{H}^m(\Omega)$  the usual Sobolev space of order  $m$  on  $\Omega$ . Then, we consider the sesquilinear form  $h^V : \mathcal{H}^1(\mathbb{R} \times \mathbb{R}_+) \times \mathcal{H}^1(\mathbb{R} \times \mathbb{R}_+) \rightarrow \mathbb{C}$  given by

$$h^V(\varphi, \psi) := \int_{\mathbb{R} \times \mathbb{R}_+} \{ \overline{(\partial_1 \varphi)(x_1, x_2)} (\partial_1 \psi)(x_1, x_2) + \overline{(\partial_2 \varphi)(x_1, x_2)} (\partial_2 \psi)(x_1, x_2) \} dx_1 dx_2 \\ + \int_{\mathbb{R}} V(x_1) \overline{\varphi(x_1, 0)} \psi(x_1, 0) dx_1,$$

where the last integral is well defined thanks to the boundary trace imbedding theorem [1, Thm. 5.36]. This sesquilinear form is lower semibounded and closed, and therefore induces in  $L^2(\mathbb{R} \times \mathbb{R}_+)$  a lower semibounded self-adjoint operator  $H^V$  with domain  $\mathcal{D}(H^V)$  satisfying the equation

$$\langle H^V \varphi, \psi \rangle_{L^2(\mathbb{R} \times \mathbb{R}_+)} = h^V(\varphi, \psi), \quad \varphi \in \mathcal{D}(H^V) \subset \mathcal{H}^1(\mathbb{R} \times \mathbb{R}_+), \quad \psi \in \mathcal{H}^1(\mathbb{R} \times \mathbb{R}_+).$$

In the case  $V \equiv 0$ , the operator  $H^0$  is the Neumann Laplacian on  $\mathbb{R} \times \mathbb{R}_+$ .

### 2.1 Direct integral decomposition of $H^V$

Let  $\mathcal{S}(\mathbb{R}^2)$  be the Schwartz space on  $\mathbb{R}^2$  and  $\mathcal{S}(\mathbb{R} \times \mathbb{R}_+) := \{ \varphi \mid \varphi = \psi|_{\mathbb{R} \times \mathbb{R}_+} \text{ for some } \psi \in \mathcal{S}(\mathbb{R}^2) \}$ . Let  $\mathbb{T} := (-\pi, \pi)$ , set  $\Pi := \mathbb{T} \times \mathbb{R}_+$ , let  $\tilde{C}^\infty(\Pi)$  be the set of functions in  $C^\infty(\Pi)$  which can be extended  $2\pi$ -periodically to functions in  $C^\infty(\mathbb{R} \times \mathbb{R}_+)$ , and for each  $m \in \mathbb{N}$  let  $\tilde{\mathcal{H}}^m(\Pi)$  be the closure of  $\tilde{C}^\infty(\Pi) \cap \mathcal{H}^m(\Pi)$  in  $\mathcal{H}^m(\Pi)$ . Then, the Gelfand transform  $\mathcal{G} : \mathcal{S}(\mathbb{R} \times \mathbb{R}_+) \rightarrow \int_{[-1/2, 1/2]}^\oplus L^2(\Pi) dk$  given by [12, Sec. 2.2]

$$(\mathcal{G}\varphi)(k, \theta, x_2) := \sum_{n \in \mathbb{Z}} e^{-ik(\theta + 2\pi n)} \varphi(\theta + 2\pi n, x_2), \quad \varphi \in \mathcal{S}(\mathbb{R} \times \mathbb{R}_+), \quad k \in [-1/2, 1/2], \quad (\theta, x_2) \in \Pi,$$

extends to a unitary operator  $\mathcal{G} : L^2(\mathbb{R} \times \mathbb{R}_+) \rightarrow \int_{[-1/2, 1/2]}^\oplus L^2(\Pi) dk$ . Moreover, one has

$$\mathcal{G} H^V \mathcal{G}^{-1} = \int_{[-1/2, 1/2]}^\oplus H_k^V dk,$$

with  $H_k^V$  the lower semibounded self-adjoint operator in  $L^2(\Pi)$  associated with the lower semibounded and closed sesquilinear form  $h_k^V : \tilde{\mathcal{H}}^1(\Pi) \times \tilde{\mathcal{H}}^1(\Pi) \rightarrow \mathbb{C}$  given by

$$h_k^V(\varphi, \psi) = \int_{\Pi} \{ \overline{((-i\partial_1 + k)\varphi)}(\theta, x_2) ((-i\partial_1 + k)\psi)(\theta, x_2) + \overline{(\partial_2 \varphi)}(\theta, x_2) (\partial_2 \psi)(\theta, x_2) \} d\theta dx_2 \\ + \int_{\mathbb{T}} V(\theta) \overline{\varphi(\theta, 0)} \psi(\theta, 0) d\theta.$$

In the case  $V \equiv 0$ , the operator  $H_k^0$  reduces to

$$H_k^0 = (P + k)^2 \otimes 1 + 1 \otimes (-\Delta_N), \quad (2.1)$$

with  $P$  the self-adjoint operator of differentiation on  $\mathbb{T}$  with periodic boundary condition and  $-\Delta_N$  the Neumann Laplacian on  $\mathbb{R}_+$ . Since  $(P + k)^2$  has purely discrete spectrum given by eigenvalues  $\lambda_{k,n} :=$

$(n+k)^2$ ,  $n \in \mathbb{Z}$ , and since  $-\Delta_N$  has purely absolutely continuous spectrum  $\sigma(-\Delta_N) = [0, \infty)$ , the operator  $H_k^0$  has purely absolutely continuous spectrum  $\sigma(H_k^0) = [k^2, \infty)$  and its spectral multiplicity is piecewise constant with a jump at each point of the threshold set

$$\tau_k := \{\lambda_{k,n}\}_{n \in \mathbb{Z}}.$$

A set of normalized eigenvectors for the operator  $(P+k)^2$  is given by the family  $\{\frac{1}{\sqrt{2\pi}} e^{in(\cdot)}\}_{n \in \mathbb{Z}} \subset L^2(\mathbb{T})$ . Since this family is independent of  $k$ , we simply write  $\{\mathcal{P}_n\}_{n \in \mathbb{Z}}$  for the corresponding set of one-dimensional orthogonal projections in  $L^2(\mathbb{T})$ .

## 2.2 Spectral representation for $H_k^0$

We now give a spectral representation of the operator  $H_k^0$  defined in (2.1) and refer to [13, Sec. 2.2] for the original representation. For that purpose, we fix  $k \in [-1/2, 1/2]$  and define the Hilbert spaces

$$\mathcal{H}_{k,n} := L^2([\lambda_{k,n}, \infty); \mathcal{P}_n L^2(\mathbb{T})) \quad \text{and} \quad \mathcal{H}_k := \bigoplus_{n \in \mathbb{Z}} \mathcal{H}_{k,n}.$$

We set  $\mathcal{S}(\mathbb{R}_+) := \{\eta \mid \eta = \zeta|_{\mathbb{R}_+} \text{ for some } \zeta \in \mathcal{S}(\mathbb{R})\}$ , we let  $\mathcal{F}_c : L^2(\mathbb{R}_+) \rightarrow L^2(\mathbb{R}_+)$  be the unitary cosine transform given by

$$(\mathcal{F}_c \eta)(y) := \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty \cos(yx) \eta(x) dx, \quad \eta \in \mathcal{S}(\mathbb{R}_+), \quad y \in \mathbb{R}_+, \quad (2.2)$$

and we let  $\mathcal{U}_k : L^2(\Pi) \rightarrow \mathcal{H}_k$  be the unitary operator given for each  $\varphi \in L^2(\mathbb{T}) \odot \mathcal{S}(\mathbb{R}_+)$  by

$$(\mathcal{U}_k \varphi)_n(\lambda) := 2^{-1/2} (\lambda - \lambda_{k,n})^{-1/4} ((\mathcal{P}_n \otimes \mathcal{F}_c) \varphi)(\cdot, \sqrt{\lambda - \lambda_{k,n}}), \quad n \in \mathbb{Z}, \quad \lambda > \lambda_{k,n}.$$

Then, the operator  $\mathcal{U}_k$  is a spectral transformation for  $H_k^0$  in the sense that  $\mathcal{U}_k H_k^0 \mathcal{U}_k^* = L_k$ , with  $L_k$  the maximal multiplication operator in  $\mathcal{H}_k$  given by

$$(L_k \xi)_n(\lambda) := \lambda \xi_n(\lambda), \quad \xi \in \mathcal{D}(L_k) := \left\{ \xi \in \mathcal{H}_k \mid \sum_{n \in \mathbb{Z}} \int_{\lambda_{k,n}}^\infty \lambda^2 \|\xi_n(\lambda)\|_{L^2(\mathbb{T})}^2 d\lambda < \infty \right\}, \quad n \in \mathbb{Z}, \quad \lambda > \lambda_{k,n}.$$

The operator  $\mathcal{U}_k$  satisfies the following regularity properties: If we define the weighted spaces

$$\mathcal{H}_s(\mathbb{R}_+) := \{\eta \in L^2(\mathbb{R}_+) \mid \langle X \rangle^s \eta \in L^2(\mathbb{R}_+)\}, \quad s \geq 0,$$

with  $X$  the maximal operator of multiplication by the variable in  $L^2(\mathbb{R}_+)$  and  $\langle x \rangle := (1+x^2)^{1/2}$ , then the operator

$$\mathcal{U}_k(n, \lambda) \varphi := (\mathcal{U}_k \varphi)_n(\lambda), \quad n \in \mathbb{Z}, \quad \lambda > \lambda_{k,n}, \quad \varphi \in L^2(\mathbb{T}) \odot \mathcal{S}(\mathbb{R}_+),$$

extends to an element of  $\mathcal{B}(L^2(\mathbb{T}) \otimes \mathcal{H}_s(\mathbb{R}_+); \mathcal{P}_n L^2(\mathbb{T}))$  for each  $s > 1/2$ , and the map

$$(\lambda_{k,n}, \infty) \ni \lambda \mapsto \mathcal{U}_k(n, \lambda) \in \mathcal{B}(L^2(\mathbb{T}) \otimes \mathcal{H}_s(\mathbb{R}_+); \mathcal{P}_n L^2(\mathbb{T}))$$

is continuous. We refer for example to [30, Prop. 2.5] for an analogue of these results on  $\mathbb{R}$  instead of  $\mathbb{R}_+$ .

## 3 Spectral analysis of $H_k^V$

In this section, we give some information on the eigenvalues of  $H_k^V$ , and we derive resolvent expansions at embedded thresholds and eigenvalues for  $H_k^V$  for any fixed value of  $k \in [-1/2, 1/2]$ .

Following the standard idea of decomposing the perturbation into factors, we define the functions

$$v : \mathbb{T} \rightarrow \mathbb{R}, \quad \theta \mapsto |V(\theta)|^{1/2} \quad \text{and} \quad u : \mathbb{T} \rightarrow \{-1, 1\}, \quad \theta \mapsto \begin{cases} 1 & \text{if } V(\theta) \geq 0 \\ -1 & \text{if } V(\theta) < 0. \end{cases}$$

Also, we use the same notation for a function and for the corresponding operator of multiplication, and we note that  $u$  is both unitary and self-adjoint as a multiplication operator in  $L^2(\mathbb{T})$ . Moreover, we set  $R_k^0(z) := (H_k^0 - z)^{-1}$  and  $R_k^V(z) := (H_k^V - z)^{-1}$  for  $z \in \mathbb{C} \setminus \mathbb{R}$ , and we define the operator  $G \in \mathcal{B}(\tilde{\mathcal{H}}^1(\Pi); L^2(\mathbb{T}))$  by

$$(G\varphi)(\theta) := v(\theta)\varphi(\theta, 0), \quad \theta \in \mathbb{T}.$$

Then, the operator  $u + GR_k^0(z)G^*$  has a bounded inverse in  $L^2(\mathbb{T})$  for each  $z \in \mathbb{C} \setminus \mathbb{R}$ , and the resolvent equation may be written as (see [12, Prop. 3.1])

$$R_k^V(z) = R_k^0(z) - R_k^0(z)G^*(u + GR_k^0(z)G^*)^{-1}GR_k^0(z), \quad z \in \mathbb{C} \setminus \mathbb{R}. \quad (3.1)$$

Alternatively, one can deduce from [31, Eq. (1.9.14)] the equivalent formula

$$GR_k^V(z)G^* = u - u(u + GR_k^0(z)G^*)^{-1}u. \quad (3.2)$$

In view of these equalities, our goal reduces to derive asymptotic expansions for the operator  $(u + GR_k^0(z)G^*)^{-1}$  as  $z \rightarrow z_0 \in \tau_k \cup \sigma_p(H_k^V)$ . For this, we first choose the square root  $\sqrt{z}$  of  $z \in \mathbb{C} \setminus [0, \infty)$  such that  $\text{Im}(\sqrt{z}) > 0$ , and then use this convention to compute explicitly the kernel of the operator  $R_k^0(z)$ :

$$(R_k^0(z))(\theta, x, \theta', x') = \frac{i}{4\pi} \sum_{n \in \mathbb{Z}} \frac{e^{in(\theta - \theta')}}{\sqrt{z - \lambda_{k,n}}} (e^{i\sqrt{z - \lambda_{k,n}}(x + x')} + e^{i\sqrt{z - \lambda_{k,n}}|x - x'|}), \quad (\theta, x), (\theta', x') \in \Pi.$$

We also refer to [12, Eq. (3.1)] for a similar formula. A straightforward computation then leads to the equality

$$GR_k^0(z)G^* = i \sum_{n \in \mathbb{Z}} \frac{v\mathcal{P}_n v}{\sqrt{z - \lambda_{k,n}}}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \quad (3.3)$$

In the sequel, we also use for  $\lambda \in [k^2, \infty)$  the definitions

$$\mathbb{Z}_k(\lambda) := \{n \in \mathbb{Z} \mid \lambda_{k,n} \leq \lambda\}, \quad \mathbb{Z}_k(\lambda)^\perp := \mathbb{Z} \setminus \mathbb{Z}_k(\lambda) \quad \text{and} \quad \beta_{k,n}(\lambda) := |\lambda - \lambda_{k,n}|^{1/4},$$

whose interest come from the following equalities:

$$GR_k^0(\lambda + i0)G^* := u\text{-}\lim_{\varepsilon \searrow 0} GR_k^0(\lambda + i\varepsilon)G^* = \sum_{n \in \mathbb{Z}_k(\lambda)^\perp} \frac{v\mathcal{P}_n v}{\beta_{k,n}(\lambda)^2} + i \sum_{n \in \mathbb{Z}_k(\lambda)} \frac{v\mathcal{P}_n v}{\beta_{k,n}(\lambda)^2}, \quad \lambda \in \mathbb{R} \setminus \tau_k, \quad (3.4)$$

where the convergence is uniform on compact subsets of  $\mathbb{R} \setminus \tau_k$ .

**Lemma 3.1.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic. Then, a value  $\lambda \in \mathbb{R} \setminus \tau_k$  is an eigenvalue of  $H_k^V$  if and only if*

$$\mathcal{K} := \ker \left( u + \sum_{n \in \mathbb{Z}_k(\lambda)^\perp} \frac{v\mathcal{P}_n v}{\beta_{k,n}(\lambda)^2} \right) \cap \left( \bigcap_{n \in \mathbb{Z}_k(\lambda)} \ker(\mathcal{P}_n v) \right) \neq \{0\},$$

and in this case the multiplicity of  $\lambda$  is equal to the dimension of  $\mathcal{K}$ .

*Proof.* We apply [31, Lemma 4.7.8]. Once the assumptions of this lemma are checked, it implies that the multiplicity of an eigenvalue  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$  is equal to the multiplicity of the eigenvalue 1 of the operator  $-GR_k^0(\lambda + i0)G^*u$ . But, the unitarity and the self-adjointness of  $u$  together with the equality (3.4) imply that the following conditions are equivalent for  $q \in L^2(\mathbb{T})$ :

$$-GR_k^0(\lambda + i0)G^*uq = q \iff uq \in \ker \left( u + \sum_{n \in \mathbb{Z}_k(\lambda)^\perp} \frac{vP_nv}{\beta_{k,n}(\lambda)^2} + i \sum_{n \in \mathbb{Z}_k(\lambda)} \frac{vP_nv}{\beta_{k,n}(\lambda)^2} \right),$$

and the second condition is in turn equivalent to the inclusion  $uq \in \mathcal{K}$ . Thus, since  $u$  is unitary we are left in proving that the assumptions of [31, Lemma 4.7.8] hold in a neighbourhood of  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$ .

Since the multiplicity of the spectrum of  $H_k^0$  is constant in each small enough neighbourhood of  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$ , it is sufficient to prove that the operators  $G$  and  $uG$  are strongly  $H_k^0$ -smooth with some exponent  $\alpha > 1/2$  on any compact subinterval of  $\mathbb{R} \setminus \tau_k$  (see [31, Def. 4.4.5] for the definition of strong  $H_0$ -smoothness). However, such a property can be checked either by using [13, Lemma 2.3] or by using the explicit formula

$$(\mathcal{U}_k G^* q)_n(\lambda) = \pi^{-1/2} \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n(vq) \in \mathcal{P}_n L^2(\mathbb{T}), \quad n \in \mathbb{Z}, \lambda > \lambda_{k,n}, q \in L^2(\mathbb{T}),$$

and the same formula with  $G^*$  replaced by  $G^*u$ .  $\square$

Lemma 3.1 has simple, but interesting, consequences on the localization of the eigenvalues of  $H_k^V$ . Indeed, one has for each  $\lambda \in \mathbb{R} \setminus \tau_k$  the inequality

$$\left\| \sum_{n \in \mathbb{Z}_k(\lambda)^\perp} \frac{vP_nv}{\beta_{k,n}(\lambda)^2} \right\| \leq \sup_{n \in \mathbb{Z}_k(\lambda)^\perp} \frac{\|V\|_\infty}{\beta_{k,n}(\lambda)^2}. \quad (3.5)$$

Therefore, if  $m \in \mathbb{Z}$  is such that  $[\lambda, \lambda_{k,m}) \cap \tau_k = \emptyset$  and  $\lambda_{k,m} - \lambda > \|V\|_\infty^2$ , one infers from (3.5) and [22, Thm. IV.1.16] that the subspace  $\mathcal{K} \equiv \mathcal{K}(\lambda)$  of Lemma 3.1 is trivial. In other words, the possible eigenvalues of  $H_k^V$  can only be located at a finite distance (independent of  $m$ ) on the left of each threshold. On the other hand, since the distance between two consecutive thresholds  $\lambda_{k,m}$  and  $\lambda_{k,m'}$  is proportional to  $|m|$ , the interval free of possible eigenvalues between two consecutive thresholds is increasing as  $|m| \rightarrow \infty$ .

**Remark 3.2.** *The above localization result is sharp. Indeed, if  $V$  is a constant function with  $V < 0$ , then we know from [14, Ex. 4.2] that  $\sigma_p(H_k^V) = \{\lambda_{k,m} - V^2 \mid m \in \mathbb{Z}\}$ .*

### 3.1 Resolvent expansions for $H_k^V$

We are now ready to derive the resolvent expansions at all points of interest by using the iterative procedure of [28, Sec. 3.1] and the associated inversion formulas. For that purpose, we set  $\mathbb{C}_+ := \{z \in \mathbb{C} \mid \text{Im}(z) > 0\}$  and we adapt a convention of [20] by considering values  $z = \lambda - \kappa^2$  with  $\kappa$  belonging to the set

$$O(\varepsilon) := \{\kappa \in \mathbb{C} \mid |\kappa| \in (0, \varepsilon), \text{Re}(\kappa) > 0 \text{ and } \text{Im}(\kappa) < 0\}, \quad \varepsilon > 0,$$

or the set

$$\tilde{O}(\varepsilon) := \{\kappa \in \mathbb{C} \mid |\kappa| \in (0, \varepsilon), \text{Re}(\kappa) \geq 0 \text{ and } \text{Im}(\kappa) \leq 0\}, \quad \varepsilon > 0.$$

Note that if  $\kappa \in O(\varepsilon)$ , then  $-\kappa^2 \in \mathbb{C}_+$  while if  $\kappa \in \tilde{O}(\varepsilon)$ , then  $-\kappa^2 \in \overline{\mathbb{C}_+}$ . With these notations at hand, the main result of this section reads as follows:

**Proposition 3.3.** *Suppose that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic, fix  $\lambda \in \tau_k \cup \sigma_p(H_k^V)$ , and take  $\kappa \in O(\varepsilon)$  with  $\varepsilon > 0$  small enough. Then, the operator  $(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1}$  belongs to  $\mathcal{B}(L^2(\mathbb{T}))$  and is continuous in the variable  $\kappa \in O(\varepsilon)$ . Moreover, the continuous function*

$$O(\varepsilon) \ni \kappa \mapsto (u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} \in \mathcal{B}(L^2(\mathbb{T}))$$

extends continuously to a function  $\tilde{O}(\varepsilon) \ni \kappa \mapsto M_\kappa(\lambda, \kappa) \in \mathcal{B}(\mathbf{L}^2(\mathbb{T}))$ , and for each  $\kappa \in \tilde{O}(\varepsilon)$  the operator  $M_\kappa(\lambda, \kappa)$  admits an asymptotic expansion in  $\kappa$ . The precise form of this expansion is given on the r.h.s. of the equations (3.14) and (3.19) below.

We recall that the relation between the asymptotic expansions given of Proposition 3.3 and the resolvent of  $H_k^V$  is given by formula (3.2). The proof of Proposition 3.3 is mainly based on an inversion formula which we reproduce here for completeness (see also [21, Prop. 1] for an earlier version):

**Proposition 3.4** (Prop. 2.1 of [28]). *Let  $O \subset \mathbb{C}$  be a subset with 0 as an accumulation point, and let  $\mathcal{H}$  be an Hilbert space. For each  $z \in O$ , let  $A(z) \in \mathcal{B}(\mathcal{H})$  satisfy*

$$A(z) = A_0 + zA_1(z),$$

with  $A_0 \in \mathcal{B}(\mathcal{H})$  and  $\|A_1(z)\|_{\mathcal{B}(\mathcal{H})}$  uniformly bounded as  $z \rightarrow 0$ . Let also  $S \in \mathcal{B}(\mathcal{H})$  be a projection such that (i)  $A_0 + S$  is invertible with bounded inverse, (ii)  $S(A_0 + S)^{-1}S = S$ . Then, for  $|z| > 0$  small enough the operator  $B(z) : S\mathcal{H} \rightarrow S\mathcal{H}$  defined by

$$B(z) := \frac{1}{z} \left( S - S(A(z) + S)^{-1}S \right) \equiv S(A_0 + S)^{-1} \left( \sum_{j \geq 0} (-z)^j (A_1(z)(A_0 + S)^{-1})^{j+1} \right) S$$

is uniformly bounded as  $z \rightarrow 0$ . Also,  $A(z)$  is invertible in  $\mathcal{H}$  with bounded inverse if and only if  $B(z)$  is invertible in  $S\mathcal{H}$  with bounded inverse, and in this case one has

$$A(z)^{-1} = (A(z) + S)^{-1} + \frac{1}{z} (A(z) + S)^{-1} S B(z)^{-1} S (A(z) + S)^{-1}.$$

*Proof of Proposition 3.3.* For each  $\lambda \in \mathbb{R}$ ,  $\varepsilon > 0$  and  $\kappa \in O(\varepsilon)$ , one has  $\text{Im}(\lambda - \kappa^2) \neq 0$ . Thus, the operator  $(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1}$  belongs to  $\mathcal{B}(\mathbf{L}^2(\mathbb{T}))$  and is continuous in  $\kappa \in O(\varepsilon)$  due to (3.1). For the other claims, we distinguish the cases  $\lambda \in \tau_k$  and  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$ , treating first the case  $\lambda \in \tau_k$ . All the operators defined below depend on the choice of  $\lambda$ , but for simplicity we do not always mention these dependencies.

(i) Assume that  $\lambda \in \tau_k$ , take  $\varepsilon > 0$ , set  $N := \{n \in \mathbb{Z} \mid \lambda_{k,n} = \lambda\}$ , and write  $\mathcal{P} := \sum_{n \in N} \mathcal{P}_n$  for the (one or two-dimensional) orthogonal projection associated with the eigenvalue  $\lambda$  of the operator  $(P+k)^2$ . Then, (3.3) implies for  $\kappa \in O(\varepsilon)$  that

$$(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} = \kappa \left\{ v\mathcal{P}v + \kappa \left( u + i \sum_{n \notin N} \frac{v\mathcal{P}_n v}{\sqrt{\lambda - \kappa^2 - \lambda_{k,n}}} \right) \right\}^{-1}.$$

Moreover, direct computations show that the function

$$O(\varepsilon) \ni \kappa \mapsto u + i \sum_{n \notin N} \frac{v\mathcal{P}_n v}{\sqrt{\lambda - \kappa^2 - \lambda_{k,n}}} \in \mathcal{B}(\mathbf{L}^2(\mathbb{T}))$$

extends continuously to a function  $\tilde{O}(\varepsilon) \ni \kappa \mapsto M_1(\kappa) \in \mathcal{B}(\mathbf{L}^2(\mathbb{T}))$  with  $\|M_1(\kappa)\|_{\mathcal{B}(\mathbf{L}^2(\mathbb{T}))}$  uniformly bounded as  $\kappa \rightarrow 0$ . Thus, one has for each  $\kappa \in O(\varepsilon)$

$$(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} = \kappa l_0(\kappa)^{-1} \quad \text{with} \quad l_0(\kappa) := v\mathcal{P}v + \kappa M_1(\kappa). \quad (3.6)$$

Now, since  $N_0 := l_0(0) = v\mathcal{P}v$  is a finite-rank operator, 0 is not a limit point of its spectrum. Also,  $N_0$  is self-adjoint, therefore the orthogonal projection  $S_0$  on  $\ker(N_0)$  is equal to the Riesz projection of  $N_0$  associated with the value 0. We can thus apply Proposition 3.4 (see [28, Cor. 2.8]), and obtain for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough that the operator  $l_1(\kappa) : S_0\mathbf{L}^2(\mathbb{T}) \rightarrow S_0\mathbf{L}^2(\mathbb{T})$  defined by

$$l_1(\kappa) := \sum_{j \geq 0} (-\kappa)^j S_0 \{ M_1(\kappa) (l_0(0) + S_0)^{-1} \}^{j+1} S_0 \quad (3.7)$$

is uniformly bounded as  $\kappa \rightarrow 0$ . Furthermore,  $l_1(\kappa)$  is invertible in  $S_0L^2(\mathbb{T})$  with bounded inverse satisfying the equation

$$l_0(\kappa)^{-1} = (l_0(\kappa) + S_0)^{-1} + \frac{1}{\kappa} (l_0(\kappa) + S_0)^{-1} S_0 l_1(\kappa)^{-1} S_0 (l_0(\kappa) + S_0)^{-1}.$$

It follows that for  $\kappa \in O(\varepsilon)$  with  $\varepsilon > 0$  small enough, one has

$$(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} = \kappa (l_0(\kappa) + S_0)^{-1} + (l_0(\kappa) + S_0)^{-1} S_0 l_1(\kappa)^{-1} S_0 (l_0(\kappa) + S_0)^{-1}, \quad (3.8)$$

with the first term vanishing as  $\kappa \rightarrow 0$ .

To describe the second term of  $(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1}$  as  $\kappa \rightarrow 0$  we note that the equality  $(l_0(0) + S_0)^{-1} S_0 = S_0$  and the definition (3.7) imply for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough that

$$l_1(\kappa) = S_0 M_1(0) S_0 + \kappa M_2(\kappa), \quad (3.9)$$

with

$$\begin{aligned} M_2(\kappa) &:= \frac{i}{\kappa} S_0 \sum_{n \notin N} \left( \frac{1}{\sqrt{\lambda - \kappa^2 - \lambda_{k,n}}} - \frac{1}{\sqrt{\lambda - \lambda_{k,n}}} \right) v \mathcal{P}_n v S_0 \\ &\quad - \sum_{j \geq 0} (-\kappa)^j S_0 \{M_1(\kappa)(l_0(0) + S_0)^{-1}\}^{j+2} S_0. \end{aligned}$$

Also, we note that the expansion

$$\frac{1}{\sqrt{\lambda - \kappa^2 - \lambda_{k,n}}} = \frac{1}{\sqrt{\lambda - \lambda_{k,n}}} \left( 1 + \frac{\kappa^2}{2(\lambda - \lambda_{k,n})} + \mathcal{O}(\kappa^4) \right), \quad n \notin N, \quad (3.10)$$

implies that  $\|M_2(\kappa)\|_{\mathcal{B}(S_0L^2(\mathbb{T}))}$  is uniformly bounded as  $\kappa \rightarrow 0$ .

Now, we have

$$M_1(0) = u + \sum_{n \in \mathbb{Z}_k(\lambda)^+} \frac{v \mathcal{P}_n v}{\beta_{k,n}(\lambda)^2} + i \sum_{n \in \mathbb{Z}_k(\lambda)^-} \frac{v \mathcal{P}_n v}{\beta_{k,n}(\lambda)^2}, \quad (3.11)$$

with  $\mathbb{Z}_k(\lambda)^- := \{n \in \mathbb{Z} \mid \lambda_{k,n} < \lambda\}$ . Therefore,  $M_1(0)$  is the sum of the unitary and self-adjoint operator  $u$ , the self-adjoint and compact operator  $\sum_{n \in \mathbb{Z}_k(\lambda)^+} \frac{v \mathcal{P}_n v}{\beta_{k,n}(\lambda)^2}$ , and the compact operator with non-negative imaginary part  $i \sum_{n \in \mathbb{Z}_k(\lambda)^-} \frac{v \mathcal{P}_n v}{\beta_{k,n}(\lambda)^2}$ . So, since  $S_0$  is an orthogonal projection with finite-dimensional kernel, the operator  $l_1(0) = S_0 M_1(0) S_0$  acting in the Hilbert space  $S_0L^2(\mathbb{T})$  can also be written as the sum of a unitary and self-adjoint operator, a self-adjoint and compact operator, and a compact operator with non-negative imaginary part. Thus, the result [28, Cor. 2.8] applies with  $S_1$  the finite-rank orthogonal projection on  $\ker(l_1(0))$ , and Proposition 3.4 can be applied to  $l_1(\kappa)$  as it was done for  $l_0(\kappa)$ .

Therefore, for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough, the operator  $l_2(\kappa) : S_1L^2(\mathbb{T}) \rightarrow S_1L^2(\mathbb{T})$  defined by

$$l_2(\kappa) := \sum_{j \geq 0} (-\kappa)^j S_1 \{M_2(\kappa)(l_1(0) + S_1)^{-1}\}^{j+1} S_1$$

is uniformly bounded as  $\kappa \rightarrow 0$ . Furthermore,  $l_2(\kappa)$  is invertible in  $S_1L^2(\mathbb{T})$  with bounded inverse satisfying the equation

$$l_1(\kappa)^{-1} = (l_1(\kappa) + S_1)^{-1} + \frac{1}{\kappa} (l_1(\kappa) + S_1)^{-1} S_1 l_2(\kappa)^{-1} S_1 (l_1(\kappa) + S_1)^{-1}.$$

This expression for  $l_1(\kappa)^{-1}$  can now be inserted in (3.8) in order to get for  $\kappa \in O(\varepsilon)$  with  $\varepsilon > 0$  small enough

$$\begin{aligned} &(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} \\ &= \kappa (l_0(\kappa) + S_0)^{-1} + (l_0(\kappa) + S_0)^{-1} S_0 (l_1(\kappa) + S_1)^{-1} S_0 (l_0(\kappa) + S_0)^{-1} \\ &\quad + \frac{1}{\kappa} (l_0(\kappa) + S_0)^{-1} S_0 (l_1(\kappa) + S_1)^{-1} S_1 l_2(\kappa)^{-1} S_1 (l_1(\kappa) + S_1)^{-1} S_0 (l_0(\kappa) + S_0)^{-1}, \end{aligned} \quad (3.12)$$

with the first two terms bounded as  $\kappa \rightarrow 0$ .

We now concentrate on the last term and check once more that the assumptions of Proposition 3.4 are satisfied. For this, we recall that  $(I_1(0) + S_1)^{-1} S_1 = S_1$ , and observe that for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough

$$I_2(\kappa) = S_1 M_2(0) S_1 + \kappa M_3(\kappa), \quad (3.13)$$

with

$$M_2(0) = -S_0 M_1(0) (I_0(0) + S_0)^{-1} M_1(0) S_0 \quad \text{and} \quad M_3(\kappa) \in \mathcal{O}(1).$$

The inclusion  $M_3(\kappa) \in \mathcal{O}(1)$  follows from simple computations taking the expansion (3.10) into account. As observed above, one has  $M_1(0) = Y + iZ^*Z$ , with  $Y, Z$  bounded self-adjoint operators in  $L^2(\mathbb{T})$ . Therefore,  $I_1(0) = S_0 M_1(0) S_0 = S_0 Y S_0 + i(Z S_0)^*(Z S_0)$ , and one infers from [28, Cor. 2.5] that  $Z S_0 S_1 = 0 = S_1 S_0 Z^*$ . Since  $S_1 S_0 = S_1 = S_0 S_1$ , it follows that  $Z S_1 = 0 = S_1 Z^*$ . Therefore, we have

$$\begin{aligned} I_2(0) &= -S_1 M_1(0) (I_0(0) + S_0)^{-1} M_1(0) S_1 \\ &= -S_1 (Y + iZ^*Z) (I_0(0) + S_0)^{-1} (Y + iZ^*Z) S_1 \\ &= -S_1 Y (I_0(0) + S_0)^{-1} Y S_1, \end{aligned}$$

and thus  $-I_2(0)$  is a positive operator.

Since  $S_1 L^2(\mathbb{T})$  is finite-dimensional, 0 is not a limit point of  $\sigma(I_2(0))$ . So, the orthogonal projection  $S_2$  on  $\ker(I_2(0))$  is a finite-rank operator, and Proposition 3.4 applies to  $I_2(0) + \kappa M_3(\kappa)$ . Thus, for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough, the operator  $I_3(\kappa) : S_2 L^2(\mathbb{T}) \rightarrow S_2 L^2(\mathbb{T})$  defined by

$$I_3(\kappa) := \sum_{j \geq 0} (-\kappa)^j S_2 \{ M_3(\kappa) (I_2(0) + S_2)^{-1} \}^{j+1} S_2$$

is uniformly bounded as  $\kappa \rightarrow 0$ . Furthermore,  $I_3(\kappa)$  is invertible in  $S_2 L^2(\mathbb{T})$  with bounded inverse satisfying the equation

$$I_2(\kappa)^{-1} = (I_2(\kappa) + S_2)^{-1} + \frac{1}{\kappa} (I_2(\kappa) + S_2)^{-1} S_2 I_3(\kappa)^{-1} S_2 (I_2(\kappa) + S_2)^{-1}.$$

This expression for  $I_2(\kappa)^{-1}$  can now be inserted in (3.12) in order to get for  $\kappa \in O(\varepsilon)$  with  $\varepsilon > 0$  small enough

$$\begin{aligned} &(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} \\ &= \kappa (I_0(\kappa) + S_0)^{-1} + (I_0(\kappa) + S_0)^{-1} S_0 (I_1(\kappa) + S_1)^{-1} S_0 (I_0(\kappa) + S_0)^{-1} \\ &\quad + \frac{1}{\kappa} (I_0(\kappa) + S_0)^{-1} S_0 (I_1(\kappa) + S_1)^{-1} S_1 (I_2(\kappa) + S_2)^{-1} S_1 (I_1(\kappa) + S_1)^{-1} S_0 (I_0(\kappa) + S_0)^{-1} \\ &\quad + \frac{1}{\kappa^2} (I_0(\kappa) + S_0)^{-1} S_0 (I_1(\kappa) + S_1)^{-1} S_1 (I_2(\kappa) + S_2)^{-1} S_2 I_3(\kappa)^{-1} S_2 (I_2(\kappa) + S_2)^{-1} S_1 \\ &\quad \times (I_1(\kappa) + S_1)^{-1} S_0 (I_0(\kappa) + S_0)^{-1}. \end{aligned} \quad (3.14)$$

Fortunately, the iterative procedure stops here. The argument is based on the relation (3.2) and the fact that  $H_k^V$  is a self-adjoint operator. Indeed, if we choose  $\kappa = \frac{\varepsilon}{2}(1 - i) \in O(\varepsilon)$ , then the inequality  $\|\kappa^2 (H_k^V - \lambda + \kappa^2)^{-1}\|_{\mathcal{B}(L^2(\mathbb{N}))} \leq 1$  holds, and thus

$$\limsup_{\kappa \rightarrow 0} \|\kappa^2 (u + GR_k^0(\lambda - \kappa^2)G^*)^{-1}\|_{\mathcal{B}(L^2(\mathbb{T}))} < \infty. \quad (3.15)$$

So, if we replace  $(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1}$  by the expression (3.14) and if we take into account that all factors of the form  $(I_j(\kappa) + S_j)^{-1}$  have a finite limit as  $\kappa \rightarrow 0$ , we infer from (3.15) that

$$\limsup_{\kappa \rightarrow 0} \|I_3(\kappa)^{-1}\|_{\mathcal{B}(S_2 L^2(\mathbb{T}))} < \infty. \quad (3.16)$$

Therefore, it only remains to show that this relation holds not just for  $\kappa = \frac{\varepsilon}{2}(1-i)$  but for all  $\kappa \in \tilde{O}(\varepsilon)$ . For that purpose, we consider  $l_3(\kappa)$  once again, and note that

$$l_3(\kappa) = S_2 M_3(0) S_2 + \kappa M_4(\kappa) \quad \text{with} \quad M_4(\kappa) \in \mathcal{O}(1). \quad (3.17)$$

The precise form of  $M_3(0)$  can be computed explicitly, but is irrelevant.

Now, since  $l_3(0)$  acts in a finite-dimensional space, 0 is an isolated eigenvalue of  $l_3(0)$  if  $0 \in \sigma(l_3(0))$ , in which case we write  $S_3$  for the corresponding Riesz projection. Then, the operator  $l_3(0) + S_3$  is invertible with bounded inverse, and (3.17) implies that  $l_3(\kappa) + S_3$  is also invertible with bounded inverse for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough. In addition, one has  $(l_3(\kappa) + S_3)^{-1} = (l_3(0) + S_3)^{-1} + \mathcal{O}(\kappa)$ . By the inversion formula given in [20, Lemma 2.1], one infers that  $S_3 - S_3(l_3(\kappa) + S_3)^{-1}S_3$  is invertible in  $S_3L^2(\mathbb{T})$  with bounded inverse and that the following equalities hold

$$\begin{aligned} l_3(\kappa)^{-1} &= (l_3(\kappa) + S_3)^{-1} + (l_3(\kappa) + S_3)^{-1} S_3 \{S_3 - S_3(l_3(\kappa) + S_3)^{-1} S_3\}^{-1} S_3 (l_3(\kappa) + S_3)^{-1} \\ &= (l_3(\kappa) + S_3)^{-1} + (l_3(\kappa) + S_3)^{-1} S_3 \{S_3 - S_3(l_3(0) + S_3)^{-1} S_3 + \mathcal{O}(\kappa)\}^{-1} S_3 (l_3(\kappa) + S_3)^{-1}. \end{aligned}$$

This implies that (3.16) holds for some  $\kappa \in \tilde{O}(\varepsilon)$  if and only if the operator  $S_3 - S_3(l_3(0) + S_3)^{-1}S_3$  is invertible in  $S_3L^2(\mathbb{T})$  with bounded inverse. But, we already know from what precedes that (3.16) holds for  $\kappa = \frac{\varepsilon}{2}(1-i)$ . So, the operator  $S_3 - S_3(l_3(0) + S_3)^{-1}S_3$  is invertible in  $S_3L^2(\mathbb{T})$  with bounded inverse, and thus (3.16) holds for all  $\kappa \in \tilde{O}(\varepsilon)$ . Therefore, (3.14) implies that the function

$$\mathcal{O}(\varepsilon) \ni \kappa \mapsto (u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} \in \mathcal{B}(L^2(\mathbb{T}))$$

extends continuously to the function  $\tilde{O}(\varepsilon) \ni \kappa \mapsto M_k(\lambda, \kappa) \in \mathcal{B}(L^2(\mathbb{T}))$ , with  $M_k(\lambda, \kappa)$  given by the r.h.s. of (3.14).

(ii) Assume that  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$ , take  $\varepsilon > 0$ , let  $\kappa \in \tilde{O}(\varepsilon)$ , and set  $J_0(\kappa) := T_0 + \kappa^2 T_1(\kappa)$  with

$$T_0 := u + \sum_{n \in \mathbb{Z}_k(\lambda)^\perp} \frac{v \mathcal{P}_n v}{\beta_{k,n}(\lambda)^2} + i \sum_{n \in \mathbb{Z}_k(\lambda)} \frac{v \mathcal{P}_n v}{\beta_{k,n}(\lambda)^2}$$

and

$$T_1(\kappa) := \frac{i}{\kappa^2} \sum_{n \in \mathbb{Z}} \left( \frac{1}{\sqrt{\lambda - \kappa^2 - \lambda_{k,n}}} - \frac{1}{\sqrt{\lambda - \lambda_{k,n}}} \right) v \mathcal{P}_n v.$$

Then, one infers from the expansion (3.10) that  $\|T_1(\kappa)\|_{\mathcal{B}(L^2(\mathbb{T}))}$  is uniformly bounded as  $\kappa \rightarrow 0$ . Also, the assumptions of [28, Cor. 2.8] hold for the operator  $T_0$ , and thus the Riesz projection  $S$  associated with the value  $0 \in \sigma(T_0)$  is an orthogonal projection. It thus follows from Proposition 3.4 that for  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough, the operator  $J_1(\kappa) : SL^2(\mathbb{T}) \rightarrow SL^2(\mathbb{T})$  defined by

$$J_1(\kappa) := \sum_{j \geq 0} (-\kappa^2)^j S \{T_1(\kappa)(T_0 + S)^{-1}\}^{j+1} S$$

is uniformly bounded as  $\kappa \rightarrow 0$ . Furthermore,  $J_1(\kappa)$  is invertible in  $SL^2(\mathbb{T})$  with bounded inverse satisfying the equation

$$J_0(\kappa)^{-1} = (J_0(\kappa) + S)^{-1} + \frac{1}{\kappa^2} (J_0(\kappa) + S)^{-1} S J_1(\kappa)^{-1} S (J_0(\kappa) + S)^{-1}.$$

It follows that for  $\kappa \in O(\varepsilon)$  with  $\varepsilon > 0$  small enough one has

$$(u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} = (J_0(\kappa) + S)^{-1} + \frac{1}{\kappa^2} (J_0(\kappa) + S)^{-1} S J_1(\kappa)^{-1} S (J_0(\kappa) + S)^{-1}. \quad (3.18)$$

Fortunately, the iterative procedure already stops here. Indeed, the argument is similar to the one presented above once we observe that

$$J_1(\kappa) = ST_1(0)S + \kappa T_2(\kappa) \quad \text{with} \quad T_2(\kappa) \in \mathcal{O}(1).$$

Therefore, (3.18) implies that the function

$$O(\varepsilon) \ni \kappa \mapsto (u + GR_k^0(\lambda - \kappa^2)G^*)^{-1} \in \mathcal{B}(L^2(\mathbb{T}))$$

extends continuously to the function  $\tilde{O}(\varepsilon) \ni \kappa \mapsto M_k(\lambda, \kappa) \in \mathcal{B}(L^2(\mathbb{T}))$ , with  $M_k(\lambda, \kappa)$  given by

$$M_k(\lambda, \kappa) = (J_0(\kappa) + S)^{-1} + \frac{1}{\kappa^2} (J_0(\kappa) + S)^{-1} S J_1(\kappa)^{-1} S (J_0(\kappa) + S)^{-1}. \quad (3.19)$$

□

The non accumulation of eigenvalues of  $H_k^V$  (except possibly at  $+\infty$ ) can easily be inferred from these asymptotic expansions (see for example [28, Corol. 3.3] in the framework of quantum waveguides). However, since such a result is already known in the present context [14, Thm. 4.1], we do not prove it again here.

We close this section with some auxiliary results which can all be deduced from the expansions of Proposition 3.3. The notations are borrowed from the proof of Proposition 3.3 (with the only change that we extend by 0 the operators defined originally on subspaces of  $L^2(\mathbb{T})$  to get operators defined on all of  $L^2(\mathbb{T})$ ). The proofs are skipped since they can be copied *mutatis mutandis* from the corresponding ones in [28, Sec. 3.1].

**Lemma 3.5.** *Take  $2 \geq \ell \geq m \geq 0$  and  $\kappa \in \tilde{O}(\varepsilon)$  with  $\varepsilon > 0$  small enough. Then, one has in  $\mathcal{B}(L^2(\mathbb{T}))$*

$$[S_\ell, (I_m(\kappa) + S_m)^{-1}] \in \mathcal{O}(\kappa).$$

Given  $\lambda \in \tau_k$ , we recall that  $N = \{n \in \mathbb{Z} \mid \lambda_{k,n} = \lambda\}$  and  $\mathcal{P} = \sum_{n \in N} \mathcal{P}_n$ .

**Lemma 3.6.** *Take  $\lambda \in \tau_k$  and let  $Y$  be the real part of the operator  $M_1(0)$ .*

- (a) *For each  $n \in N$ , one has  $\mathcal{P}_n \nu S_0 = 0 = S_0 \nu \mathcal{P}_n$ .*
- (b) *For each  $n \in \mathbb{Z}_k(\lambda)$ , one has  $\mathcal{P}_n \nu S_1 = 0 = S_1 \nu \mathcal{P}_n$ .*
- (c) *One has  $Y S_2 = 0 = S_2 Y$ .*
- (d) *One has  $M_1(0) S_2 = 0 = S_2 M_1(0)$ .*

## 4 Continuity properties of the scattering matrix

We prove in this section continuity properties of the channel scattering matrices associated with the scattering pair  $\{H_k^0, H_k^V\}$ . As before, the value of  $k \in [-1/2, 1/2]$  is fixed throughout the section.

First, we note that under the assumption that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic the wave operators

$$W_{k,\pm} := s\text{-}\lim_{t \rightarrow \pm\infty} e^{itH_k^V} e^{-itH_k^0}$$

exist and are complete (see [12, Thm. 2.1]). As a consequence, the scattering operator

$$S_k := W_{k,+}^* W_{k,-}$$

is a unitary operator in  $L^2(\Pi)$  which commutes with  $H_k^0$ , and thus  $S_k$  is decomposable in the spectral representation of  $H_k^0$ . To give an explicit formula for  $S_k$  in that representation, that is, for the operator  $\mathcal{U}_k S_k \mathcal{U}_k^*$  in  $\mathcal{H}_k$ , we recall from Proposition 3.3, Lemma 3.1, and formula (3.4), that the operator

$$\mathbf{M}_k(\lambda, 0) \equiv \lim_{\varepsilon \searrow 0} (u + GR_k^0(\lambda + i\varepsilon)G^*)^{-1} \quad (4.1)$$

belongs to  $\mathcal{B}(L^2(\mathbb{T}))$  for each  $\lambda \in [k^2, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\}$ . We also define for  $n, n' \in \mathbb{Z}$  the operator  $\delta_{nn'} \in \mathcal{B}(\mathcal{P}_{n'} L^2(\mathbb{T}); \mathcal{P}_n L^2(\mathbb{T}))$  by  $\delta_{nn'} = 1$  if  $n = n'$  and  $\delta_{nn'} = 0$  otherwise. Then, a computation using stationary formulas as presented in [31, Sec. 2.8] shows that

$$(\mathcal{U}_k S_k \mathcal{U}_k^* \xi)_n(\lambda) := \sum_{n' \in \mathbb{Z}_k(\lambda)} S_k(\lambda)_{nn'} \xi_{n'}(\lambda), \quad \xi \in \mathcal{H}_k, \quad n \in \mathbb{Z}, \quad \lambda \in [\lambda_{k,n}, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\},$$

with  $S_k(\lambda)_{nn'}$  the channel scattering matrix given by

$$S_k(\lambda)_{nn'} = \delta_{nn'} - 2i\beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu \mathbf{M}_k(\lambda, 0) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda)^{-1}. \quad (4.2)$$

Moreover, the explicit formula (3.4) implies for each  $n, n' \in \mathbb{Z}$  the continuity of the map

$$[k^2, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\} \ni \lambda \mapsto S_k(\lambda)_{nn'} \in \mathcal{B}(\mathcal{P}_{n'} L^2(\mathbb{T}), \mathcal{P}_n L^2(\mathbb{T})), \quad \lambda_{k,n}, \lambda_{k,n'} < \lambda.$$

Therefore, in order to completely determine the continuity properties of the channel scattering matrices  $S_k(\lambda)_{nn'}$ , it only remains to describe the behaviour of  $S_k(\lambda)_{nn'}$  as  $\lambda \rightarrow \lambda_0 \in \tau_k \cup \sigma_p(H_k^V)$ . In the sequel, we consider separately the behaviour of  $S_k(\lambda)_{nn'}$  at thresholds and at embedded eigenvalues, starting with the thresholds.

For that purpose, we first note that for each  $\lambda \in \tau_k$ , a channel can either be already open (in which case one has to show the existence and the equality of the limits from the right and from the left), or can open at the energy  $\lambda$  (in which case one has only to show the existence of the limit from the right). Therefore, as in the previous section, we shall fix  $\lambda \in \tau_k$ , and consider the expression  $S_k(\lambda - \kappa^2)_{nn'}$  for suitable  $\kappa$  with  $|\kappa| > 0$  small enough (recall that all expressions of Section 3 were also computed at fixed  $\lambda \in \tau_k$  but that the dependence on  $\lambda$  has not been explicitly written for the simplicity).

Before considering the continuity at thresholds, we define for each fixed  $\lambda \in \tau_k$ , for  $\kappa \in \tilde{\mathcal{O}}(\varepsilon)$  with  $\varepsilon > 0$  small enough, and for  $2 \geq \ell \geq m \geq 0$  the operators

$$C_{\ell m}(\kappa) := [S_\ell, (I_m(\kappa) + S_m)^{-1}] \in \mathcal{B}(L^2(\mathbb{T})),$$

and note that  $C_{\ell m}(\kappa) \in \mathcal{O}(\kappa)$  due to Lemma 3.5. In fact, the formulas (3.6), (3.9) and (3.13) imply that  $C'_{\ell m}(0) := \lim_{\kappa \rightarrow 0} \frac{1}{\kappa} C_{\ell m}(\kappa)$  exists in  $\mathcal{B}(L^2(\mathbb{T}))$ . In other cases, we use the notation  $F(\kappa) \in \mathcal{O}_{\text{as}}(\kappa^n)$ ,  $n \in \mathbb{N}$ , for an operator  $F(\kappa) \in \mathcal{O}(\kappa^n)$  such that  $\lim_{\kappa \rightarrow 0} \kappa^{-n} F(\kappa)$  exists in  $\mathcal{B}(L^2(\mathbb{T}))$ . We also note that if  $\kappa \in (0, \varepsilon)$  or  $i\kappa \in (0, \varepsilon)$  with  $\varepsilon > 0$ , then  $\kappa \in \tilde{\mathcal{O}}(\varepsilon)$  and  $-\kappa^2 \in (-\varepsilon^2, \varepsilon^2) \setminus \{0\}$ .

**Theorem 4.1.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic, let  $\lambda \in \tau_k$ , take  $\kappa \in (0, \varepsilon)$  or  $i\kappa \in (0, \varepsilon)$  with  $\varepsilon > 0$  small enough, and let  $n, n' \in \mathbb{Z}$ .*

(a) *If  $\lambda_{k,n}, \lambda_{k,n'} < \lambda$ , then the limit  $\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'}$  exists and is given by*

$$\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'} = \delta_{nn'} - 2i\beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu S_0 (I_1(0) + S_1)^{-1} S_0 \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda)^{-1}.$$

(b) *If  $\lambda_{k,n}, \lambda_{k,n'} \leq \lambda$  and  $-\kappa^2 > 0$ , then the limit  $\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'}$  exists and is given by*

$$\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'} = \begin{cases} 0 & \text{if } \lambda_{k,n} < \lambda, \lambda_{k,n'} = \lambda, \\ 0 & \text{if } \lambda_{k,n} = \lambda, \lambda_{k,n'} < \lambda, \\ \delta_{nn'} - 2\mathcal{P}_n \nu (I_0(0) + S_0)^{-1} \nu \mathcal{P}_{n'} & \\ \quad + 2\mathcal{P}_n \nu C'_{10}(0) S_1 (I_2(0) + S_2)^{-1} S_1 C'_{10}(0) \nu \mathcal{P}_{n'} & \text{if } \lambda_{k,n} = \lambda = \lambda_{k,n'}. \end{cases}$$

Before the proof, we note that the r.h.s. of (3.14) can be rewritten as in [28, Sec. 3.3]:

$$\begin{aligned}
& \mathbf{M}_k(\lambda, \kappa) \\
&= \kappa(l_0(\kappa) + S_0)^{-1} \\
&+ \left( S_0(l_0(\kappa) + S_0)^{-1} - C_{00}(\kappa) \right) S_0(l_1(\kappa) + S_1)^{-1} S_0 \left( (l_0(\kappa) + S_0)^{-1} S_0 + C_{00}(\kappa) \right) \\
&+ \frac{1}{\kappa} \left\{ \left( S_1(l_0(\kappa) + S_0)^{-1} - C_{10}(\kappa) \right) (l_1(\kappa) + S_1)^{-1} - \left( S_0(l_0(\kappa) + S_0)^{-1} - C_{00}(\kappa) \right) C_{11}(\kappa) \right\} \\
&\quad \times S_1(l_2(\kappa) + S_2)^{-1} S_1 \left\{ (l_1(\kappa) + S_1)^{-1} \left( (l_0(\kappa) + S_0)^{-1} S_1 + C_{10}(\kappa) \right) \right. \\
&\quad \left. + C_{11}(\kappa) \left( (l_0(\kappa) + S_0)^{-1} S_0 + C_{00}(\kappa) \right) \right\} \\
&+ \frac{1}{\kappa^2} \left\{ \left[ \left( S_2(l_0(\kappa) + S_0)^{-1} - C_{20}(\kappa) \right) (l_1(\kappa) + S_1)^{-1} \right. \right. \\
&\quad \left. \left. - \left( S_0(l_0(\kappa) + S_0)^{-1} - C_{00}(\kappa) \right) C_{21}(\kappa) \right] (l_2(\kappa) + S_2)^{-1} \right. \\
&\quad \left. - \left[ \left( S_1(l_0(\kappa) + S_0)^{-1} - C_{10}(\kappa) \right) (l_1(\kappa) + S_1)^{-1} \right. \right. \\
&\quad \left. \left. - \left( S_0(l_0(\kappa) + S_0)^{-1} - C_{00}(\kappa) \right) C_{11}(\kappa) \right] C_{22}(\kappa) \right\} S_2 l_3(\kappa)^{-1} S_2 \\
&\quad \times \left\{ (l_2(\kappa) + S_2)^{-1} \left[ (l_1(\kappa) + S_1)^{-1} \left( (l_0(\kappa) + S_0)^{-1} S_2 + C_{20}(\kappa) \right) \right. \right. \\
&\quad \left. \left. + C_{21}(\kappa) \left( (l_0(\kappa) + S_0)^{-1} S_0 + C_{00}(\kappa) \right) \right] \right. \\
&\quad \left. + C_{22}(\kappa) \left[ (l_1(\kappa) + S_1)^{-1} \left( (l_0(\kappa) + S_0)^{-1} S_1 + C_{10}(\kappa) \right) \right. \right. \\
&\quad \left. \left. + C_{11}(\kappa) \left( (l_0(\kappa) + S_0)^{-1} S_0 + C_{00}(\kappa) \right) \right] \right\}. \tag{4.3}
\end{aligned}$$

The interest in this formulation is that the projections  $S_\ell$  (which lead to simplifications in the proof below) have been put into evidence at the beginning or at the end of each term.

*Proof.* (a) Some lengthy, but direct, computations taking into account the expansion (4.3), the relation  $(l_\ell(0) + S_\ell)^{-1} S_\ell = S_\ell$ , the expansion

$$\beta_{k,n}(\lambda - \kappa^2)^{-1} = \beta_{k,n}(\lambda)^{-1} \left( 1 + \frac{\kappa^2}{4(\lambda - \lambda_{k,n})} + \mathcal{O}(\kappa^4) \right), \quad \lambda_{k,n} < \lambda, \tag{4.4}$$

and Lemma 3.6(b) lead to the equality

$$\begin{aligned}
& \lim_{\kappa \rightarrow 0} \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu \mathbf{M}_k(\lambda, \kappa) \nu \mathcal{P}_n' \beta_{k,n}(\lambda - \kappa^2)^{-1} \\
&= \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu S_0(l_1(0) + S_1)^{-1} S_0 \nu \mathcal{P}_n' \beta_{k,n}(\lambda)^{-1} \\
&\quad - \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu (C'_{20}(0) + S_0 C'_{21}(0)) S_2 l_3(0)^{-1} S_2 (C'_{20}(0) + C'_{21}(0) S_0) \nu \mathcal{P}_n' \beta_{k,n}(\lambda)^{-1}.
\end{aligned}$$

Moreover, Lemmas 3.6(a) and 3.6(d) imply that

$$\begin{aligned}
C_{20}(\kappa) &= (l_0(\kappa) + S_0)^{-1} [\nu \mathcal{P} \nu + \kappa M_1(\kappa), S_2] (l_0(\kappa) + S_0)^{-1} \\
&= \kappa (l_0(0) + S_0)^{-1} [M_1(0), S_2] (l_0(0) + S_0)^{-1} + \mathcal{O}_{\text{as}}(\kappa^2) \\
&= \mathcal{O}_{\text{as}}(\kappa^2), \tag{4.5}
\end{aligned}$$

and Lemma 3.6(d) and the expansion (3.10) imply that

$$\begin{aligned}
C_{21}(\kappa) &= (I_1(\kappa) + S_1)^{-1} [S_0 M_1(0) S_0 + \kappa M_2(\kappa), S_2] (I_1(\kappa) + S_1)^{-1} \\
&= \kappa (I_1(\kappa) + S_0)^{-1} [M_2(\kappa), S_2] (I_1(\kappa) + S_0)^{-1} \\
&= \kappa (I_1(\kappa) + S_0)^{-1} [-S_0 M_1(0) (I_0(0) + S_0)^{-1} M_1(0) S_0, S_2] (I_1(\kappa) + S_0)^{-1} + \mathcal{O}_{\text{as}}(\kappa^2) \\
&= \mathcal{O}_{\text{as}}(\kappa^2).
\end{aligned}$$

Therefore, one has  $C'_{20}(0) = C'_{21}(0) = 0$ , and thus

$$\begin{aligned}
&\lim_{\kappa \rightarrow 0} \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu M_k(\lambda, \kappa) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1} \\
&= \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu S_0 (I_1(0) + S_1)^{-1} S_0 \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda)^{-1}.
\end{aligned}$$

Since

$$S_k(\lambda - \kappa^2)_{nn'} - \delta_{nn'} = -2i \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu M_k(\lambda, \kappa) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1}, \quad (4.6)$$

this proves the claim.

(b.1) We first consider the case  $\lambda_{k,n} < \lambda$ ,  $\lambda_{k,n'} = \lambda$  (the case  $\lambda_{k,n} = \lambda$ ,  $\lambda_{k,n'} < \lambda$  is not presented since it is similar). An inspection of the expansion (4.3) taking into account the relation  $(I_\ell(\kappa) + S_\ell)^{-1} = (I_\ell(0) + S_\ell)^{-1} + \mathcal{O}_{\text{as}}(\kappa)$  and the relation  $(I_\ell(0) + S_\ell)^{-1} S_\ell = S_\ell$  leads to the equation

$$\begin{aligned}
&\beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu M_k(\lambda, \kappa) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1} \\
&= \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu \left\{ \mathcal{O}_{\text{as}}(\kappa) + S_0 (I_1(\kappa) + S_1)^{-1} S_0 \right. \\
&\quad + \frac{1}{\kappa} (S_1 + \mathcal{O}_{\text{as}}(\kappa)) S_1 (I_2(\kappa) + S_2)^{-1} S_1 (S_1 + \mathcal{O}_{\text{as}}(\kappa)) \\
&\quad + \frac{1}{\kappa^2} \left[ \mathcal{O}_{\text{as}}(\kappa^2) + S_2 (I_0(\kappa) + S_0)^{-1} (I_1(\kappa) + S_1)^{-1} (I_2(\kappa) + S_2)^{-1} - C_{20}(\kappa) - S_0 C_{21}(\kappa) - S_1 C_{22}(\kappa) \right] \\
&\quad \times S_2 I_3(\kappa)^{-1} S_2 \left[ \mathcal{O}_{\text{as}}(\kappa^2) + (I_2(\kappa) + S_2)^{-1} (I_1(\kappa) + S_1)^{-1} (I_0(\kappa) + S_0)^{-1} S_2 + C_{20}(\kappa) + C_{21}(\kappa) S_0 \right. \\
&\quad \left. \left. + C_{22}(\kappa) S_1 \right] \right\} \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1}.
\end{aligned}$$

An application of Lemma 3.6(a)-(b) to the previous equation gives

$$\begin{aligned}
&\beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu M_k(\lambda, \kappa) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1} \\
&= \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu \left\{ \mathcal{O}_{\text{as}}(\kappa) - \frac{1}{\kappa^2} (\mathcal{O}_{\text{as}}(\kappa^2) + C_{20}(\kappa) + S_0 C_{21}(\kappa)) S_2 I_3(\kappa)^{-1} S_2 (\mathcal{O}_{\text{as}}(\kappa^2) + C_{20}(\kappa)) \right\} \\
&\quad \times \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1}.
\end{aligned}$$

Finally, if one takes into account the expansion (4.4) for  $\beta_{k,n}(\lambda - \kappa^2)^{-1}$  and the equality  $\beta_{k,n'}(\lambda - \kappa^2)^{-1} = |\kappa|^{-1/2}$ , one ends up with

$$\begin{aligned}
&\beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu M_k(\lambda, \kappa) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1} \\
&= -\frac{1}{\kappa^2 |\kappa|^{1/2}} \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu (C_{20}(\kappa) + S_0 C_{21}(\kappa)) S_2 I_3(\kappa)^{-1} S_2 C_{20}(\kappa) \nu \mathcal{P}_{n'} + \mathcal{O}(|\kappa|^{1/2}).
\end{aligned}$$

Since  $C_{20}(\kappa) = \mathcal{O}_{\text{as}}(\kappa^2)$  (see (4.5)), one infers that  $\beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n \nu M_k(\lambda, \kappa) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1}$  vanishes as  $\kappa \rightarrow 0$ , and thus that the limit  $\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'}$  also vanishes due to (4.6).

(b.2) We are left with the case  $\lambda_{k,n} = \lambda = \lambda_{k,n'}$ . An inspection of the expansion (4.3) taking into account the relation  $(I_\ell(\kappa) + S_\ell)^{-1} = (I_\ell(0) + S_\ell)^{-1} + \mathcal{O}_{\text{as}}(\kappa)$ , the relation  $(I_\ell(0) + S_\ell)^{-1} S_\ell = S_\ell$  and

Lemma 3.6(a) leads to the equation

$$\begin{aligned} & \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n v \mathbf{M}_k(\lambda, \kappa) v \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1} \\ &= \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n v \left\{ \mathcal{O}_{\text{as}}(\kappa^2) + \kappa(l_0(\kappa) + S_0)^{-1} - \frac{1}{\kappa} C_{10}(\kappa) S_1 (l_2(\kappa) + S_2)^{-1} S_1 C_{10}(\kappa) \right. \\ & \quad \left. - \frac{1}{\kappa^2} (\mathcal{O}_{\text{as}}(\kappa^2) + C_{20}(\kappa)) S_2 l_3(\kappa)^{-1} S_2 (\mathcal{O}_{\text{as}}(\kappa^2) + C_{20}(\kappa)) \right\} v \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1}. \end{aligned}$$

Therefore, since  $\beta_{k,n}(\lambda - \kappa^2)^{-1} = \beta_{k,n'}(\lambda - \kappa^2)^{-1} = |\kappa|^{-1/2}$  and  $C_{20}(\kappa) \in \mathcal{O}_{\text{as}}(\kappa^2)$ , one obtains that

$$\begin{aligned} & \lim_{\kappa \rightarrow 0} \beta_{k,n}(\lambda - \kappa^2)^{-1} \mathcal{P}_n v \mathbf{M}_k(\lambda, \kappa) v \mathcal{P}_{n'} \beta_{k,n'}(\lambda - \kappa^2)^{-1} \\ &= -i \mathcal{P}_n v (l_0(0) + S_0)^{-1} v \mathcal{P}_{n'} + i \mathcal{P}_n v C'_{10}(0) S_1 (l_2(0) + S_2)^{-1} S_1 C'_{10}(0) v \mathcal{P}_{n'}, \end{aligned}$$

and thus that

$$\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'} = \delta_{nn'} - 2 \mathcal{P}_n v (l_0(0) + S_0)^{-1} v \mathcal{P}_{n'} + 2 \mathcal{P}_n v C'_{10}(0) S_1 (l_2(0) + S_2)^{-1} S_1 C'_{10}(0) v \mathcal{P}_{n'}$$

due to (4.6).  $\square$

We finally consider the continuity of the scattering matrix at embedded eigenvalues not located at thresholds.

**Theorem 4.2.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic, take  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$ ,  $\kappa \in (0, \varepsilon)$  or  $i\kappa \in (0, \varepsilon)$  with  $\varepsilon > 0$  small enough, and let  $n, n' \in \mathbb{Z}$ . Then, if  $\lambda_{k,n}, \lambda_{k,n'} < \lambda$ , the limit  $\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'}$  exists and is given by*

$$\lim_{\kappa \rightarrow 0} S_k(\lambda - \kappa^2)_{nn'} = \delta_{nn'} - 2i \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n v (J_0(0) + S)^{-1} v \mathcal{P}_{n'} \beta_{k,n'}(\lambda)^{-1} \quad (4.7)$$

*Proof.* We know from (3.19) that

$$\mathbf{M}_k(\lambda, \kappa) = (J_0(\kappa) + S)^{-1} + \frac{1}{\kappa^2} (J_0(\kappa) + S)^{-1} S J_1(\kappa)^{-1} S (J_0(\kappa) + S)^{-1},$$

with  $S$  the Riesz projection associated with the value 0 of the operator

$$T_0 = u + \sum_{m \in \mathbb{Z}_k(\lambda)^\perp} \frac{v \mathcal{P}_m v}{\beta_{k,m}(\lambda)^2} + i \sum_{m \in \mathbb{Z}_k(\lambda)} \frac{v \mathcal{P}_m v}{\beta_{k,m}(\lambda)^2}.$$

Now, since  $J_0(\kappa) = T_0 + \kappa^2 T_1(\kappa)$  with  $T_1(\kappa) \in \mathcal{O}_{\text{as}}(1)$ , a commutation of  $S$  with  $(J_0(\kappa) + S)^{-1}$  gives

$$\mathbf{M}_k(\lambda, \kappa) = (J_0(\kappa) + S)^{-1} + \frac{1}{\kappa^2} \{S (J_0(\kappa) + S)^{-1} + \mathcal{O}_{\text{as}}(\kappa^2)\} S J_1(\kappa)^{-1} S \{(J_0(\kappa) + S)^{-1} S + \mathcal{O}_{\text{as}}(\kappa^2)\}.$$

In addition, an application of [28, Lemma 2.5] shows that  $\mathcal{P}_n v S = 0 = S v \mathcal{P}_n$  for each  $n \in \mathbb{Z}_k(\lambda)$ . These relations, together with (4.6), imply the equality (4.7).  $\square$

## 5 Structure of the wave operators

In this section, we establish new stationary formulas for the wave operators  $W_{k,\pm}$  for a fixed value of  $k \in [-1/2, 1/2]$ , and also for the full wave operators  $W_\pm(H^0, H^V)$ . As before, we assume throughout the section that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic.

We recall from [31, Eq. 2.7.5] that  $W_{k,-}$  satisfies for suitable  $\varphi, \psi \in L^2(\Pi)$  the following equation:

$$\langle W_{k,-} \varphi, \psi \rangle_{L^2(\Pi)} = \int_{\mathbb{R}} d\lambda \lim_{\varepsilon \searrow 0} \frac{\varepsilon}{\pi} \langle R_k^0(\lambda - i\varepsilon) \varphi, R_k^V(\lambda - i\varepsilon) \psi \rangle_{L^2(\Pi)}.$$

We also recall from [31, Sec. 1.4] that if  $\delta_\varepsilon(H_k^0 - \lambda) := \frac{\pi^{-1}\varepsilon}{(H_k^0 - \lambda)^2 + \varepsilon^2}$  for  $\varepsilon > 0$ , then the limit  $\lim_{\varepsilon \searrow 0} \langle \delta_\varepsilon(H_k^0 - \lambda) \varphi, \psi \rangle_{L^2(\Pi)}$  exists for a.e.  $\lambda \in \mathbb{R}$  and verifies

$$\langle \varphi, \psi \rangle_{L^2(\Pi)} = \int_{\mathbb{R}} d\lambda \lim_{\varepsilon \searrow 0} \langle \delta_\varepsilon(H_k^0 - \lambda) \varphi, \psi \rangle_{L^2(\Pi)}.$$

So, by taking (3.1) into account and by using the fact that  $\lim_{\varepsilon \searrow 0} \|\delta_\varepsilon(H_k^0 - \lambda)\|_{\mathcal{B}(L^2(\Pi))} = 0$  if  $\lambda < k^2$ , one infers that

$$\langle (W_{k,-} - 1) \varphi, \psi \rangle_{L^2(\Pi)} = - \int_{k^2}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \langle G^* M_k(\lambda + i\varepsilon) G \delta_\varepsilon(H_k^0 - \lambda) \varphi, R_k^0(\lambda - i\varepsilon) \psi \rangle_{L^2(\Pi)},$$

with

$$M_k(z) := (u + G R_k^0(z) G^*)^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Below, we derive an expression for the operator  $(W_{k,-} - 1)$  in the spectral representation of  $H_k^0$ ; that is, for the operator  $\mathcal{U}_k(W_{k,-} - 1)\mathcal{U}_k^*$ . For that purpose, we decompose the operator  $G$  into the product  $G = v \gamma_0$ , with  $\gamma_0 \in \mathcal{B}(\tilde{\mathcal{H}}^1(\Pi); L^2(\mathbb{T}))$  given by

$$(\gamma_0 \varphi)(\theta) := \varphi(\theta, 0), \quad \varphi \in \tilde{\mathcal{H}}^1(\Pi), \theta \in \mathbb{T}.$$

We also define the set

$$\mathcal{D}_k := \left\{ \xi \in \mathcal{H}_k \mid \xi_n = \rho_n \otimes e^{in(\cdot)}, \rho_n \in C_c^\infty((\lambda_{k,n}, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\}), \right. \\ \left. \rho_n \neq 0 \text{ for a finite number of } n \in \mathbb{Z} \right\}$$

which is dense in  $\mathcal{H}_k$  since the point spectrum of  $H_k^V$  has no accumulation point except possibly at  $+\infty$ . Finally, we give the short following lemma, which will be useful in the subsequent computations for the wave operators.

**Lemma 5.1.** *For  $\xi \in \mathcal{D}_k$  and  $\lambda \geq k^2$ , one has*

$$(a) \quad \gamma_0 \mathcal{U}_k^* \xi = \pi^{-1/2} \sum_{n \in \mathbb{Z}} \int_{\lambda_{k,n}}^{\infty} d\mu \beta_{k,n}(\mu)^{-1} \xi_n(\mu) \in L^2(\mathbb{T}),$$

$$(b) \quad s\text{-}\lim_{\varepsilon \searrow 0} \gamma_0 \mathcal{U}_k^* \delta_\varepsilon(L_k - \lambda) \xi = \pi^{-1/2} \sum_{n \in \mathbb{Z}_k(\lambda)} \beta_{k,n}(\lambda)^{-1} \xi_n(\lambda) \in L^2(\mathbb{T}).$$

*Proof.* The equality in (a) follows from a direct computation, and the inclusion in  $L^2(\mathbb{T})$  follows from the fact that  $\mathcal{U}_k^* \xi \in \tilde{\mathcal{H}}^1(\Pi)$ . For (b), it is sufficient to note that the map  $\mu \mapsto \beta_{k,n}(\mu)^{-1} \xi_n(\mu)$  extends trivially to a continuous function on  $\mathbb{R}$  with compact support in  $(\lambda_{k,n}, \infty)$ , and then to use the convergence of the Dirac delta sequence  $\delta_\varepsilon(\cdot - \lambda)$ .  $\square$

Thus, if we let  $\xi, \zeta \in \mathcal{D}_k$  and take the previous observations into account, we obtain the equalities

$$\begin{aligned}
& \langle \mathcal{W}_k(W_{k,-} - 1) \mathcal{W}_k^* \xi, \zeta \rangle_{\mathcal{H}_k} \\
&= - \int_{k^2}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \langle \gamma_0^* v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{W}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \mathcal{W}_k^*(L_k - \lambda + i\varepsilon)^{-1} \zeta \rangle_{L^2(\Pi)} \\
&= - \int_{k^2}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \langle v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{W}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \gamma_0 \mathcal{W}_k^*(L_k - \lambda + i\varepsilon)^{-1} \zeta \rangle_{L^2(\mathbb{T})} \\
&= - \int_{k^2}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{W}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \sum_{n \in \mathbb{Z}} \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \\
&= - \sum_{n \in \mathbb{Z}} \int_{\lambda_{k,n}}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{W}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \quad (5.1)
\end{aligned}$$

$$- \sum_{n \in \mathbb{Z}} \int_{k^2}^{\lambda_{k,n}} d\lambda \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{W}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \quad (5.2)$$

with the sums over  $n$  being finite. In the next two sections, we study separately the terms (5.1) and (5.2).

## 5.1 Wave operators: the leading term

We prove in this section an explicit formula for the term (5.1) in the expression for  $(W_{k,-} - 1)$  in terms of the generator of dilations in  $\mathbb{R}_+$ . For this, we recall that the dilation group  $\{U_\tau^+\}_{\tau \in \mathbb{R}}$  in  $L^2(\mathbb{R}_+)$  is defined by

$$(U_\tau^+ \varphi)(\lambda) := e^{\tau/2} \varphi(e^\tau \lambda), \quad \varphi \in C_c(\mathbb{R}_+), \lambda \in \mathbb{R}_+, \tau \in \mathbb{R},$$

and that the self-adjoint generator of  $\{U_\tau^+\}_{\tau \in \mathbb{R}}$  is denoted by  $A_+$ .

**Proposition 5.2.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic and take  $\xi, \zeta \in \mathcal{D}_k$ . Then, we have*

$$\begin{aligned}
& - \sum_{n \in \mathbb{Z}} \int_{\lambda_{k,n}}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{W}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \\
&= \langle \mathcal{W}_k(1 \otimes R(A_+))(S_k - 1) \mathcal{W}_k^* \xi, \zeta \rangle_{\mathcal{H}_k}
\end{aligned}$$

with

$$R(x) := \frac{1}{2} (1 + \tanh(\pi x) + i \cosh(\pi x)^{-1}), \quad x \in \mathbb{R}. \quad (5.3)$$

*Proof.* (i) Take  $\eta \in C_c^\infty(\mathbb{R}_+)$  and  $x \in \mathbb{R}_+$ , let  $\mathcal{F}$  be the Fourier transform on  $\mathbb{R}$ , and write  $\chi_+$  for the characteristic function for  $\mathbb{R}_+$ . Then, we have

$$\begin{aligned}
(\Theta \eta)(x) &:= 2 \int_0^\infty dy \int_0^\infty dz x e^{i(y^2 - x^2)z} \eta(y) \\
&= 2^{3/2} \pi^{1/2} \int_0^\infty dy (\mathcal{F}^* \chi_+)(y^2 - x^2) x \eta(y) \\
&= 2^{3/2} \pi^{1/2} \int_{\mathbb{R}} dz (\mathcal{F}^* \chi_+)(x^2(e^{2z} - 1)) x^2 e^z \eta(e^z x) \quad (y = e^z x) \\
&= 2^{3/2} \pi^{1/2} \int_{\mathbb{R}} dz (\mathcal{F}^* \chi_+)(x^2(e^{2z} - 1)) x^2 e^{z/2} (U_z^+ \eta)(x).
\end{aligned}$$

Then, by using the fact that  $\mathcal{F}^* \chi_+ = 2^{-1/2} \pi^{1/2} \delta_0 + i(2\pi)^{-1/2} \text{Pv} \frac{1}{(\cdot)}$  with  $\delta_0$  the Dirac delta distribution

and Pv the principal value, one gets that

$$\begin{aligned} (\Theta\eta)(x) &= 2 \int_{\mathbb{R}} dz \left( \pi \delta_0(e^{2z} - 1) + i \operatorname{Pv} \frac{e^{z/2}}{e^{2z} - 1} \right) (U_z^+ \eta)(x) \\ &= \int_{\mathbb{R}} dz \left( \pi \delta_0(z) + \frac{i}{2} \operatorname{Pv} \left( \frac{1}{\sinh(z/2)} - \frac{1}{\cosh(z/2)} \right) \right) (U_z^+ \eta)(x). \end{aligned}$$

So, by taking into account the equality [18, Table 20.1]

$$(2\pi)^{1/2} (\mathcal{F}\bar{R})(z) = \pi \delta_0(-z) + \frac{i}{2} \operatorname{Pv} \left( \frac{1}{\sinh(-z/2)} - \frac{1}{\cosh(-z/2)} \right)$$

with  $R$  as in (5.3), one infers that

$$(\Theta\eta)(x) = (2\pi)^{1/2} \int_{\mathbb{R}} dz (\mathcal{F}\bar{R})(-z) (U_z^+ \eta)(x) = 2\pi (\bar{R}(-A_+) \eta)(x).$$

Therefore, one has for each  $\zeta \in \mathcal{D}_k$ ,  $n \in \mathbb{Z}$  and  $\lambda > \lambda_{k,n}$  the following equalities in  $L^2(\mathbb{T})$ :

$$\begin{aligned} & 2\pi (\mathcal{U}_k(1 \otimes \bar{R}(A_+)) \mathcal{U}_k^* \zeta)_n(\lambda) \\ &= 2\pi (\mathcal{U}_k(1 \otimes \mathcal{F}_c^* \bar{R}(-A_+) \mathcal{F}_c) \mathcal{U}_k^* \zeta)_n(\lambda) \\ &= (\mathcal{U}_k(1 \otimes \mathcal{F}_c^* \Theta \mathcal{F}_c) \mathcal{U}_k^* \zeta)_n(\lambda) \\ &= 2^{-1/2} (\lambda - \lambda_{k,n})^{-1/4} ((\mathcal{P}_n \otimes \Theta \mathcal{F}_c) \mathcal{U}_k^* \zeta)(\cdot, (\lambda - \lambda_{k,n})^{1/2}) \\ &= 2^{1/2} (\lambda - \lambda_{k,n})^{-1/4} \int_0^\infty dy \int_0^\infty dz (\lambda - \lambda_{k,n})^{1/2} e^{i(y^2 - \lambda + \lambda_{k,n})z} ((\mathcal{P}_n \otimes \mathcal{F}_c) \mathcal{U}_k^* \zeta)(\cdot, y) \\ &= 2(\lambda - \lambda_{k,n})^{1/4} \int_0^\infty dy \int_0^\infty dz e^{i(y^2 - \lambda + \lambda_{k,n})z} y^{1/2} \zeta_n(y^2 + \lambda_{k,n}) \\ &= \int_{\lambda_{k,n}}^\infty d\mu \int_0^\infty dz e^{i(\mu - \lambda)z} \beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1} \zeta_n(\mu). \end{aligned} \tag{5.4}$$

(ii) Let  $\xi, \zeta \in \mathcal{D}_k$  and take  $\varepsilon > 0$ ,  $n \in \mathbb{Z}$  and  $\lambda \in [\lambda_{k,n}, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\}$ . Then, Lemma 5.1(a), the formula  $(\mu - \lambda + i\varepsilon)^{-1} = -i \int_0^\infty dz e^{i(\mu - \lambda)z} e^{-\varepsilon z}$  and Fubini's theorem imply that

$$\begin{aligned} & \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} \nu M_k(\lambda + i\varepsilon) \nu \gamma_0 \mathcal{U}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^\infty d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \\ &= \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu M_k(\lambda + i\varepsilon) \nu \gamma_0 \mathcal{U}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^\infty d\mu \frac{\beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \\ &= \lim_{\varepsilon \searrow 0} \int_0^\infty dz e^{-\varepsilon z} \left\langle g_\varepsilon(n, \lambda), \int_{\lambda_{k,n}}^\infty d\mu e^{i(\mu - \lambda)z} \beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \end{aligned} \tag{5.5}$$

with

$$g_\varepsilon(n, \lambda) := i\pi^{-1} \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu M_k(\lambda + i\varepsilon) \nu \sum_{n' \in \mathbb{Z}} \int_{\lambda_{k,n'}}^\infty d\nu \beta_{k,n'}(\nu)^{-1} \delta_\varepsilon(\nu - \lambda) \xi_{n'}(\nu).$$

Now, we already know from (4.1) that  $\lim_{\varepsilon \searrow 0} M_k(\lambda + i\varepsilon) = M_k(\lambda, 0)$  in  $\mathcal{B}(L^2(\mathbb{T}))$  and we have

$$\operatorname{s-lim}_{\varepsilon \searrow 0} \sum_{n' \in \mathbb{Z}} \int_{\lambda_{k,n'}}^\infty d\nu \beta_{k,n'}(\nu)^{-1} \delta_\varepsilon(\nu - \lambda) \xi_{n'}(\nu) = \sum_{n' \in \mathbb{Z}_k(\lambda)} \beta_{k,n'}(\lambda)^{-1} \xi_{n'}(\lambda)$$

in  $L^2(\mathbb{T})$ . Therefore, we have

$$g_0(n, \lambda) := \operatorname{s-lim}_{\varepsilon \searrow 0} g_\varepsilon(n, \lambda) = i\pi^{-1} \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu M_k(\lambda, 0) \nu \sum_{n' \in \mathbb{Z}_k(\lambda)} \beta_{k,n'}(\lambda)^{-1} \xi_{n'}(\lambda)$$

in  $L^2(\mathbb{T})$ , and the integrand in (5.5) can be bounded independently of  $\varepsilon \in (0, 1)$ :

$$\begin{aligned} & \left| e^{-\varepsilon z} \left\langle g_\varepsilon(n, \lambda), \int_{\lambda_{k,n}}^{\infty} d\mu e^{i(\mu-\lambda)z} \beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \right| \\ & \leq \text{Const.} \left\| \int_{\lambda_{k,n}}^{\infty} d\mu e^{i(\mu-\lambda)z} \beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1} \zeta_n(\mu) \right\|_{L^2(\mathbb{T})}. \end{aligned} \quad (5.6)$$

In order to exchange the integral over  $z$  and the limit  $\varepsilon \searrow 0$  in (5.5), it remains to show that the r.h.s. of (5.6) belongs to  $L^1(\mathbb{R}_+, dz)$ . For that purpose, we note that

$$\begin{aligned} \left\| \int_{\lambda_{k,n}}^{\infty} d\mu e^{i(\mu-\lambda)z} \beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1} \zeta_n(\mu) \right\|_{L^2(\mathbb{T})} &= \left\| \int_{\lambda_{k,n}-\lambda}^{\infty} d\nu e^{i\nu z} \beta_{k,n}(\lambda) \beta_{k,n}(\nu+\lambda)^{-1} \zeta_n(\nu+\lambda) \right\|_{L^2(\mathbb{T})} \\ &= \left\| (\mathcal{F}^* h_{n,\lambda})(z) \right\|_{L^2(\mathbb{T})} \end{aligned}$$

with  $h_{n,\lambda}$  the trivial extension of the function

$$(\lambda_{k,n} - \lambda, \infty) \ni \nu \mapsto (2\pi)^{1/2} \beta_{k,n}(\lambda) \beta_{k,n}(\nu + \lambda)^{-1} \zeta_n(\nu + \lambda) \in L^2(\mathbb{T})$$

to all of  $\mathbb{R}$ . Then, writing  $P$  for the self-adjoint operator  $-i\nabla$  on  $\mathbb{R}$ , and using the fact that

$$h_{n,\lambda}(\nu) = \begin{cases} (2\pi)^{1/2} \beta_{k,n}(\lambda) \beta_{k,n}(\nu + \lambda)^{-1} \rho_n(\nu + \lambda) e^{i\nu(\cdot)} & \text{if } \nu > \lambda_{k,n} - \lambda \\ 0 & \text{if } \nu \leq \lambda_{k,n} - \lambda \end{cases}$$

with  $\rho_n \in C_c^\infty((\lambda_{k,n}, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\})$ , one obtains that

$$\left\| (\mathcal{F}^* h_{n,\lambda})(z) \right\|_{L^2(\mathbb{T})} = \langle z \rangle^{-2} \left\| (\mathcal{F}^* \langle P \rangle^2 h_{n,\lambda})(z) \right\|_{L^2(\mathbb{T})} \leq \text{Const.} \langle z \rangle^{-2}, \quad z \in \mathbb{R}_+.$$

As a consequence, one can apply Lebesgue dominated convergence theorem and Fubini's theorem to infer that (5.5) is equal to

$$\left\langle g_0(n, \lambda), \int_{\lambda_{k,n}}^{\infty} d\mu \int_0^{\infty} dz e^{i(\mu-\lambda)z} \beta_{k,n}(\lambda) \beta_{k,n}(\mu)^{-1} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})}.$$

This, together with (4.2) and (5.4), implies that

$$\begin{aligned} & \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} \nu M_k(\lambda + i\varepsilon) \nu \gamma_0 \mathcal{U}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \\ &= \left\langle \sum_{n' \in \mathbb{Z}_k(\lambda)} 2i \beta_{k,n}(\lambda)^{-1} \mathcal{P}_n \nu M_k(\lambda, 0) \nu \mathcal{P}_{n'} \beta_{k,n'}(\lambda)^{-1} \xi_{n'}(\lambda), (\mathcal{U}_k(1 \otimes \bar{R}(A_+)) \mathcal{U}_k^* \zeta)_n(\lambda) \right\rangle_{L^2(\mathbb{T})} \\ &= -\langle (\mathcal{U}_k(S_k - 1) \mathcal{U}_k^* \xi)_n(\lambda), (\mathcal{U}_k(1 \otimes \bar{R}(A_+)) \mathcal{U}_k^* \zeta)_n(\lambda) \rangle_{L^2(\mathbb{T})}. \end{aligned}$$

Now, the last equality holds not only for  $\lambda \in [\lambda_{k,n}, \infty) \setminus \{\tau_k \cup \sigma_p(H_k^V)\}$  but for all  $\lambda \in [\lambda_{k,n}, \infty)$ , since for each  $n \in \mathbb{Z}$  and all  $\lambda \in \tau_k \cup \sigma_p(H_k^V)$  we have  $\xi_n(\lambda) = 0$ . So, we finally obtain that

$$\begin{aligned} & - \sum_{n \in \mathbb{Z}} \int_{\lambda_{k,n}}^{\infty} d\lambda \lim_{\varepsilon \searrow 0} \left\langle \pi^{-1/2} \nu M_k(\lambda + i\varepsilon) \nu \gamma_0 \mathcal{U}_k^* \delta_\varepsilon(L_k - \lambda) \xi, \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{L^2(\mathbb{T})} \\ &= \langle \mathcal{U}_k(1 \otimes R(A_+))(S_k - 1) \mathcal{U}_k^* \xi, \zeta \rangle_{\mathcal{H}_k}, \end{aligned}$$

as desired.  $\square$

## 5.2 Wave operators: the remainder term

We prove in this section that the remaining term (5.2) in the expression for  $(W_{k,-} - 1)$  can be written as a matrix operator in  $\mathcal{H}_k$  with Hilbert-Schmidt components. For this, we start with a lemma which complements the continuity properties obtained Section 4.

**Lemma 5.3.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic, and choose  $n, n' \in \mathbb{Z}$  such that  $\lambda_{k,n'} < \lambda_{k,n}$ . Then, the function*

$$[\lambda_{k,n'}, \lambda_{k,n}] \setminus \{\tau_k \cup \sigma_p(H_k^V)\} \ni \lambda \mapsto \beta_{k,n}(\lambda)^{-2} \mathcal{P}_n v M_k(\lambda, 0) v \mathcal{P}_{n'} \in \mathcal{B}(L^2(\mathbb{T})) \quad (5.7)$$

extends to a continuous function on  $[\lambda_{k,n'}, \lambda_{k,n}]$ .

*Proof.* Since the function (5.7) is continuous on  $[\lambda_{k,n'}, \lambda_{k,n}] \setminus \{\tau_k \cup \sigma_p(H_k^V)\}$ , one only has to check that the function admits limits in  $\mathcal{B}(L^2(\mathbb{T}))$  as  $\lambda \rightarrow \lambda_0 \in \{\tau_k \cup \sigma_p(H_k^V)\}$ . However, in order to be able to use the asymptotic expansions of Proposition 3.3, we slightly change the point of view by considering values  $\lambda - \kappa^2 \in \mathbb{C}$  with  $\lambda \in \{\tau_k \cup \sigma_p(H_k^V)\}$  and  $\kappa \rightarrow 0$  in a suitable domain of  $\mathbb{C}$  of diameter  $\varepsilon > 0$ . Namely, we consider the three following possible cases: when  $\lambda = \lambda_{k,n'}$  and  $i\kappa \in (0, \varepsilon)$  (case 1), when  $\lambda = \lambda_{k,n}$  and  $\kappa \in (0, \varepsilon)$  (case 2), and when  $\lambda \in (\lambda_{k,n'}, \lambda_{k,n}) \cap \{\tau_k \cup \sigma_p(H_k^V)\}$  and  $\kappa \in (0, \varepsilon)$  or  $i\kappa \in (0, \varepsilon)$  (case 3). In each case, we choose  $\varepsilon > 0$  small enough so that  $\{z \in \mathbb{C} \mid |z| < \varepsilon\} \cap \{\tau_k \cup \sigma_p(H_k^V)\} = \{\lambda\}$  (this is possible because  $\tau_k$  is discrete and  $\sigma_p(H_k^V)$  has no accumulation point).

(i) First, assume that  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$  and let  $\kappa \in (0, \varepsilon)$  or  $i\kappa \in (0, \varepsilon)$  with  $\varepsilon > 0$  small enough. Then, we know from (3.19) that

$$\mathcal{P}_n v M_k(\lambda, \kappa) v \mathcal{P}_{n'} = \mathcal{P}_n v (J_0(\kappa) + S)^{-1} v \mathcal{P}_{n'} + \frac{1}{\kappa^2} \mathcal{P}_n v (J_0(\kappa) + S)^{-1} S J_1(\kappa)^{-1} S (J_0(\kappa) + S)^{-1} v \mathcal{P}_{n'}$$

with  $S$ ,  $J_0(\kappa)$  and  $J_1(\kappa)$  as in point (ii) of the proof of Proposition 3.3. Furthermore, point (ii) of the proof of Proposition 3.3 implies that  $[S, J_0(\kappa)] \in \mathcal{O}_{as}(\kappa^2)$ , and Lemma 3.6(b) (applied with  $S$  instead of  $S_1$ ) implies that  $S v \mathcal{P}_{n'} = 0$ . Therefore,

$$\begin{aligned} \mathcal{P}_n v M_k(\lambda, \kappa) v \mathcal{P}_{n'} &= \mathcal{O}_{as}(1) + \frac{1}{\kappa^2} \mathcal{P}_n v (J_0(\kappa) + S)^{-1} S J_1(\kappa)^{-1} S \{(J_0(\kappa) + S)^{-1} S + \mathcal{O}_{as}(\kappa^2)\} v \mathcal{P}_{n'} \\ &= \mathcal{O}_{as}(1). \end{aligned}$$

Since  $\lim_{\kappa \rightarrow 0} \beta_{k,n}(\lambda - \kappa^2)^{-2} = |\lambda - \lambda_{k,n}|^{-1/2} < \infty$  for each  $\lambda \in \sigma_p(H_k^V) \setminus \tau_k$ , we thus infer that the function (5.7) (with  $\lambda$  replaced by  $\lambda - \kappa^2$ ) admits a limit in  $\mathcal{B}(L^2(\mathbb{T}))$  as  $\kappa \rightarrow 0$ .

(ii) Now, assume that  $\lambda \in [\lambda_{k,n'}, \lambda_{k,n}] \cap \tau_k$ , and consider the three above cases simultaneously. For this, we recall that  $i\kappa \in (0, \varepsilon)$  in case 1,  $\kappa \in (0, \varepsilon)$  in case 2, and  $\kappa \in (0, \varepsilon)$  or  $i\kappa \in (0, \varepsilon)$  in case 3. Also, we note that the factor  $\beta_{k,n}(\lambda - \kappa^2)^{-2}$  does not play any role in cases 1 and 3, but gives a singularity of order  $|\kappa|^{-1}$  in case 2.

In the expansion (4.3), the first term (the one linear in  $\kappa$ ) admits a limit in  $\mathcal{B}(L^2(\mathbb{T}))$  as  $\kappa \rightarrow 0$ , even in case 2. For the second term (the one of order  $\mathcal{O}_{as}(1)$  in  $\kappa$ ) only case 2 requires a special attention: in this case, the existence of the limit as  $\kappa \rightarrow 0$  follows from the inclusion  $C_{00}(\kappa) \in \mathcal{O}_{as}(\kappa)$  and the equality  $\mathcal{P}_n v S_0 = 0$ , which holds by Lemma 3.6(a). For the third term (the one with prefactor  $\frac{1}{\kappa}$ ), in cases 1 and 3, it is sufficient to observe that  $C_{00}(\kappa), C_{10}(\kappa) \in \mathcal{O}_{as}(\kappa)$  and that  $S_1 v \mathcal{P}_{n'} = 0$  by Lemma 3.6(b). On the other hand, for case 2, one must take into account the inclusions  $C_{00}(\kappa), C_{10}(\kappa) \in \mathcal{O}_{as}(\kappa)$ , the equality  $S_1 v \mathcal{P}_{n'} = 0$  of Lemma 3.6(b) and the equality  $\mathcal{P}_n v S_1 = 0$  of Lemma 3.6(a). For the fourth term (the one with prefactor  $\frac{1}{\kappa^2}$ ), in cases 1 and 3, it is sufficient to observe that  $C_{20}(\kappa), C_{21}(\kappa) \in \mathcal{O}_{as}(\kappa^2)$  and that  $S_2 v \mathcal{P}_{n'} = 0 = S_1 v \mathcal{P}_{n'}$ . On the other hand, for case 2, one must take into account the inclusions  $C_{20}(\kappa), C_{21}(\kappa) \in \mathcal{O}_{as}(\kappa^2)$ , the equalities  $S_2 v \mathcal{P}_{n'} = 0 = S_1 v \mathcal{P}_{n'}$ , and the equality  $\mathcal{P}_n v S_2 = 0$ .  $\square$

Now, to obtain the desired formula for the term (5.2), we define for  $\varepsilon > 0$ ,  $n \in \mathbb{Z}$ ,  $\lambda \in \mathbb{R}$  and  $\xi \in \mathcal{D}_k$  the vector

$$g_\varepsilon(n, \lambda) := \pi^{-1/2} \mathcal{P}_n v M_k(\lambda + i\varepsilon) v \gamma_0 \mathcal{U}_k^* \delta_\varepsilon(L_k - \lambda) \xi \in L^2(\mathbb{T}),$$

and we note from Proposition 3.3 and Lemma 5.1(b) that for each  $\lambda \in (k^2, \lambda_{k,n}) \setminus \{\tau_k \cup \sigma_p(H_k^V)\}$  we have

$$g_0(n, \lambda) := \text{s-lim}_{\varepsilon \searrow 0} g_\varepsilon(n, \lambda) = \pi^{-1} \mathcal{P}_n \nu \mathbf{M}(\lambda, 0) \nu \sum_{n' \in \mathbb{Z}_k(\lambda)} \beta_{k,n'}(\lambda)^{-1} \xi_{n'}(\lambda).$$

Then, we observe that (5.2) can be written as

$$- \sum_{n \in \mathbb{Z}} \int_{k^2}^{\lambda_{k,n}} d\lambda \lim_{\varepsilon \searrow 0} \left\langle g_\varepsilon(n, \lambda), \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{\mathbb{L}^2(\mathbb{T})} \quad (5.8)$$

with

$$\left| \left\langle g_\varepsilon(n, \lambda), \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\rangle_{\mathbb{L}^2(\mathbb{T})} \right| \leq \text{Const.} \left\| \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\mu)^{-1}}{\mu - \lambda + i\varepsilon} \zeta_n(\mu) \right\|_{\mathbb{L}^2(\mathbb{T})}.$$

Since the r.h.s. can be bounded independently of  $\varepsilon$ , we infer from Lebesgue dominated convergence theorem that (5.8) can be rewritten as

$$- \sum_{n \in \mathbb{Z}} \sum_{n' \in \mathbb{Z}_k(\lambda_{k,n})} \int_{\lambda_{k,n'}}^{\lambda_{k,n}} d\lambda \left\langle B_{nn'}(\lambda) \xi_{n'}(\lambda), \int_{\lambda_{k,n}}^{\infty} d\mu \frac{\beta_{k,n}(\lambda)^2 \beta_{k,n}(\mu)^{-1} \beta_{k,n'}(\lambda)^{-1}}{\pi(\mu - \lambda)} \zeta_n(\mu) \right\rangle_{\mathbb{L}^2(\mathbb{T})} \quad (5.9)$$

with

$$B_{nn'}(\lambda) = \beta_{k,n}(\lambda)^{-2} \mathcal{P}_n \nu \mathbf{M}_k(\lambda, 0) \nu \mathcal{P}_{n'} \in \mathcal{B}(\mathbb{L}^2(\mathbb{T})) \quad \text{for a.e. } \lambda \in (\lambda_{k,n'}, \lambda_{k,n}). \quad (5.10)$$

But the map  $\lambda \mapsto B_{nn'}(\lambda)$  coincides with the map (5.7). Therefore, Lemma 5.3 and Fubini's theorem imply that (5.9) can be written as  $\langle Q_k \xi, \zeta \rangle_{\mathcal{H}_k}$ , with  $Q_k : \mathcal{H}_k \rightarrow \mathcal{H}_k$  given for  $\xi \in \mathcal{D}_k$ ,  $n \in \mathbb{Z}$  and  $\mu > \lambda_{k,n}$  by

$$(Q_k \xi)_n(\mu) := - \sum_{n' \in \mathbb{Z}_k(\lambda_{k,n})} \int_{\lambda_{k,n'}}^{\lambda_{k,n}} d\lambda \frac{\beta_{k,n}(\lambda)^2 \beta_{k,n}(\mu)^{-1} \beta_{k,n'}(\lambda)^{-1}}{\pi(\mu - \lambda)} B_{nn'}(\lambda) \xi_{n'}(\lambda).$$

To simplify the last formula, we define the operator  $B_{nn'} \in \mathcal{B}(\mathcal{H}_{k,n'}; \mathbb{L}^2((\lambda_{k,n'}, \lambda_{k,n}); \mathcal{P}_n \mathbb{L}^2(\mathbb{T})))$  by

$$(B_{nn'} \xi_{n'})_n(\lambda) := B_{nn'}(\lambda) \xi_{n'}(\lambda) \quad \text{for a.e. } \lambda \in (\lambda_{k,n'}, \lambda_{k,n}).$$

We also define the integral operator  $C_{nn'} : \mathbb{L}^2((\lambda_{k,n'}, \lambda_{k,n}); \mathcal{P}_n \mathbb{L}^2(\mathbb{T})) \rightarrow \mathcal{H}_{k,n}$  with kernel

$$C_{nn'}(\mu, \lambda) := \frac{\beta_{k,n}(\lambda)^2 \beta_{k,n}(\mu)^{-1} \beta_{k,n'}(\lambda)^{-1}}{\pi(\mu - \lambda)}, \quad \mu > \lambda_{k,n}, \lambda \in (\lambda_{k,n'}, \lambda_{k,n}),$$

and show that  $C_{nn'}$  is a Hilbert-Schmidt operator.

**Lemma 5.4.** *The operator  $C_{nn'}$  is a Hilbert-Schmidt operator from  $\mathbb{L}^2((\lambda_{k,n'}, \lambda_{k,n}); \mathcal{P}_n \mathbb{L}^2(\mathbb{T}))$  to  $\mathcal{H}_{k,n}$ .*

*Proof.* Using the changes of variables  $x := (\mu - \lambda_{k,n})^{1/2}$ ,  $y := (\lambda_{k,n} - \lambda)^{1/2}$ , and the notation  $\alpha := (\lambda_{k,n} - \lambda_{k,n'})^{1/2}$ , one obtains that

$$\begin{aligned} & \int_{\lambda_{k,n}}^{\infty} d\mu \int_{\lambda_{k,n'}}^{\lambda_{k,n}} d\lambda \frac{|\lambda - \lambda_{k,n}| |\mu - \lambda_{k,n}|^{-1/2} |\lambda - \lambda_{k,n'}|^{-1/2}}{\pi^2(\mu - \lambda)^2} \\ &= \frac{4}{\pi^2} \int_0^\infty dx \int_0^\alpha dy \frac{y^3 (\alpha^2 - y^2)^{-1/2}}{(x^2 + y^2)^2} \\ &= \frac{4}{\pi^2} \int_0^\alpha dy \frac{y^3}{(\alpha^2 - y^2)^{1/2}} \left( \frac{x}{2y^2(x^2 + y^2)} + \frac{\arctan(x/y)}{2y^3} \right) \Big|_{x=0}^{x=\infty} \\ &= \frac{1}{\pi} \int_0^\alpha dy (\alpha^2 - y^2)^{-1/2} \\ &= 1/2. \end{aligned}$$

It follows that  $C_{nn'}$  is a Hilbert-Schmidt operator from  $\mathbb{L}^2((\lambda_{k,n'}, \lambda_{k,n}); \mathcal{P}_n \mathbb{L}^2(\mathbb{T}))$  to  $\mathcal{H}_{k,n}$  with Hilbert-Schmidt norm equal to  $1/\sqrt{2}$ .  $\square$

Therefore, the remainder term (5.2) in the expression for  $(W_{k,-} - 1)$  can be written as  $\langle Q_k \xi, \zeta \rangle_{\mathcal{H}_k}$  with  $Q_k : \mathcal{H}_k \rightarrow \mathcal{H}_k$  given by

$$(Q_k \xi)_n = - \sum_{r \in \mathbb{Z}_k(\lambda_{k,n})} C_{nr'} B_{nr'} \xi_{r'}, \quad \xi \in \mathcal{D}_k, \quad n \in \mathbb{Z}, \quad (5.11)$$

where each summand  $C_{nr'} B_{nr'} : \mathcal{H}_{k,r'} \rightarrow \mathcal{H}_{k,n}$  belongs to the Hilbert-Schmidt class.

We close the section with two observations which show that the remainder term  $Q_k$  is always small in some suitable sense. First, we consider the case of a constant function  $V$  :

**Remark 5.5.** *If the function  $V$  is constant, then the remainder term  $Q_k$  vanishes. Indeed, in such a case one can easily check that the operator  $M_k(\lambda, 0)$  is diagonal in the basis  $\{\frac{1}{\sqrt{2\pi}} e^{in(\cdot)}\}_{n \in \mathbb{Z}} \subset L^2(\mathbb{T})$ . As a result, one obtains that  $B_{nr'}(\lambda) = 0$ , which in turn implies that  $Q_k = 0$  (see (5.10) and (5.11)).*

Second, we consider the case of a general function  $V$  :

**Lemma 5.6.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic. Then, the remainder term  $Q_k$  vanishes asymptotically along the free evolution, that is,*

$$\text{s-lim}_{t \rightarrow \pm\infty} e^{itH_k^0} \mathcal{U}_k^* Q_k \mathcal{U}_k e^{-itH_k^0} = 0 \quad \text{in } L^2(\Pi).$$

*Proof.* The equations (5.1)-(5.2), Proposition 5.2 and the results of this section imply that

$$\langle \mathcal{U}_k (W_{k,-} - 1) \mathcal{U}_k^* \xi, \zeta \rangle_{\mathcal{H}_k} = \langle \mathcal{U}_k (1 \otimes R(A_+)) (S_k - 1) \mathcal{U}_k^* \xi, \zeta \rangle_{\mathcal{H}_k} + \langle Q_k \xi, \zeta \rangle_{\mathcal{H}_k}, \quad \xi, \zeta \in \mathcal{D}_k.$$

Therefore, we deduce from the density of  $\mathcal{D}_k$  in  $\mathcal{H}_k$  and the unitarity of  $\mathcal{U}_k : L^2(\Pi) \rightarrow \mathcal{H}_k$  that

$$W_{k,-} - 1 - (1 \otimes R(A_+)) (S_k - 1) = \mathcal{U}_k^* Q_k \mathcal{U}_k. \quad (5.12)$$

Also, we know from the existence and completeness of the wave operators  $W_{k,\pm}$  that

$$\text{s-lim}_{t \rightarrow \pm\infty} e^{itH_k^0} S_k e^{-itH_k^0} = S_k, \quad \text{s-lim}_{t \rightarrow \infty} e^{itH_k^0} W_{k,-} e^{-itH_k^0} = S_k \quad \text{and} \quad \text{s-lim}_{t \rightarrow -\infty} e^{itH_k^0} W_{k,-} e^{-itH_k^0} = 1. \quad (5.13)$$

Furthermore, the definition of the function  $R$  (see (5.3)) and Proposition 6.1 imply in  $L^2(\mathbb{R}_+)$  the relations

$$\text{s-lim}_{t \rightarrow \infty} e^{it(-\Delta_N)} R(A_+) e^{-it(-\Delta_N)} = 1 \quad \text{and} \quad \text{s-lim}_{t \rightarrow -\infty} e^{it(-\Delta_N)} R(A_+) e^{-it(-\Delta_N)} = 0,$$

which in turn imply in  $L^2(\Pi)$  the relations

$$\text{s-lim}_{t \rightarrow \infty} e^{itH_k^0} (1 \otimes R(A_+)) e^{-itH_k^0} = 1 \quad \text{and} \quad \text{s-lim}_{t \rightarrow -\infty} e^{itH_k^0} (1 \otimes R(A_+)) e^{-itH_k^0} = 0. \quad (5.14)$$

Then, one can conclude by combining the equations (5.12)-(5.14).  $\square$

### 5.3 New formula for the wave operators

In this final section, we collect the information on the wave operators obtained so far.

**Lemma 5.7.** *Assume that  $V \in L^\infty(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic. Then, we have in  $L^2(\Pi)$  the equalities*

$$W_{k,-} - 1 = (1 \otimes R(A_+)) (S_k - 1) + \mathcal{U}_k^* Q_k \mathcal{U}_k \quad (5.15)$$

and

$$W_{k,+} - 1 = (1 - 1 \otimes R(A_+)) (S_k^* - 1) + \mathcal{U}_k^* Q_k \mathcal{U}_k S_k^*, \quad (5.16)$$

with  $R$  and  $Q_k$  given in (5.3) and (5.11). In addition, the term  $Q_k$  satisfies

$$\text{s-lim}_{t \rightarrow \pm\infty} e^{itH_k^0} \mathcal{U}_k^* Q_k \mathcal{U}_k e^{-itH_k^0} = 0.$$

*Proof.* As already mentioned in the proof of Lemma 5.6, the equations (5.1)-(5.2), Proposition 5.2 and the results of Section 5.2 imply the formula (5.15) for  $W_{k,-}$ . The formula (5.16) for  $W_{k,+}$  follows from (5.15) and from the relation  $W_{k,+} = W_{k,-} S_k^*$ . Finally, the properties of the term  $Q_k$  follow directly from Lemma 5.6.  $\square$

Now, we know from [12, Sec. 2.4] that the wave operators  $W_{\pm} \equiv W_{\pm}(H^0, H^V)$  and the scattering operator  $S \equiv S(H^0, H^V)$  for the pair  $\{H^0, H^V\}$  admit direct integral decompositions

$$\mathcal{G} W_{\pm} \mathcal{G}^{-1} = \int_{[-1/2, 1/2]}^{\oplus} W_{k, \pm} dk \quad \text{and} \quad \mathcal{G} S \mathcal{G}^{-1} = \int_{[-1/2, 1/2]}^{\oplus} S_k dk,$$

with  $\mathcal{G} : L^2(\mathbb{R} \times \mathbb{R}_+) \rightarrow \int_{[-1/2, 1/2]}^{\oplus} L^2(\Pi) dk$  the Gelfand transform of Section 2.1. Therefore, one directly infers from Lemma 5.7 the following new formulas for  $W_{\pm}$  :

**Theorem 5.8.** *Assume that  $V \in L^{\infty}(\mathbb{R}; \mathbb{R})$  is  $2\pi$ -periodic. Then, we have in  $L^2(\mathbb{R} \times \mathbb{R}_+)$  the equalities*

$$W_- - 1 = (1 \otimes R(A_+))(S - 1) + Q \quad \text{and} \quad W_+ - 1 = (1 - 1 \otimes R(A_+))(S^* - 1) + QS^*,$$

with  $Q := \mathcal{G}^{-1} \left( \int_{[-1/2, 1/2]}^{\oplus} \mathcal{U}_k^* Q_k \mathcal{U}_k dk \right) \mathcal{G}$ .

## 6 Appendix

We present in this appendix a proposition of independent interest on the asymptotic behaviour of functions of the generator of dilations  $A_+$  under the time evolution generated by the Neumann Laplacian  $-\Delta_N$ . Before this, we recall that the usual weighted  $L^2$ -spaces are defined by

$$\mathcal{H}_t(\mathbb{R}) := \left\{ \varphi \in L^2(\mathbb{R}) \mid \int_{\mathbb{R}} (1 + |x|^2)^t |\varphi(x)|^2 < \infty \right\}, \quad t \geq 0.$$

**Proposition 6.1.** *Let  $f \in C^1(\mathbb{R})$  satisfy  $f' \in \mathcal{H}_t(\mathbb{R})$  for some  $t > 1/2$  and  $\lim_{x \rightarrow \pm\infty} f(x) = f_{\pm}$  for some  $f_{\pm} \in \mathbb{C}$ . Then, one has*

$$\text{s-lim}_{t \rightarrow \pm\infty} e^{it(-\Delta_N)} f(A_+) e^{-it(-\Delta_N)} = f_{\pm}. \quad (6.1)$$

*Proof.* The operator of multiplication in  $L^2(\mathbb{R}_+)$  given by

$$(B\varphi)(x) := \frac{1}{2} \ln(x^2) \varphi(x), \quad \varphi \in C_c^{\infty}(\mathbb{R}_+),$$

is essentially self-adjoint [25, Ex. 5.1.15], with self-adjoint extension denoted by the same symbol. Also, a direct calculation shows that  $B$  and  $A_+$  satisfy for  $t \in \mathbb{R}$  and  $\varphi \in C_c^{\infty}(\mathbb{R}_+)$  the relation

$$e^{itB} A_+ e^{-itB} \varphi = (A_+ - t) \varphi.$$

Since  $C_c^{\infty}(\mathbb{R}_+)$  is a core for  $A_+$ , this implies that  $e^{itB} A_+ e^{-itB} = (A_+ - t)$  as self-adjoint operators. Therefore, one obtains that

$$\text{s-lim}_{t \rightarrow \pm\infty} e^{itB} f(A_+) e^{-itB} = \text{s-lim}_{t \rightarrow \pm\infty} f(e^{itB} A_+ e^{-itB}) = \text{s-lim}_{t \rightarrow \pm\infty} f(A_+ - t) = f_{\mp}.$$

Now, one can apply to the last relation the invariance principle for wave operators as presented in [4, Sec. 16.1.1] to obtain for each  $\eta \in C_c^{\infty}(\mathbb{R})$  the relation

$$\text{s-lim}_{t \rightarrow \pm\infty} e^{it e^{2B}} f(A_+) e^{-it e^{2B}} \eta(B) = f_{\mp} \eta(B). \quad (6.2)$$

For this, one has to check that the function  $x \mapsto e^{2x}$  is admissible in the sense of [4, Def. 8.1.16] and that the commutator  $Bf(A_+)\eta(B) - f(A_+)\eta(B)B$ , defined as a quadratic form on  $\mathcal{D}(B)$ , extends to a trace class operator. The first condition is trivially verified. For the second condition, we have the following equalities in the form sense on  $C_c^\infty(\mathbb{R}_+)$  :

$$\begin{aligned} Bf(A_+)\eta(B) - f(A_+)\eta(B)B &= -i \left( s - \frac{d}{dt} e^{itB} f(A_+) e^{-itB} \right)_{t=0} \eta(B) \\ &= -i \left( s - \frac{d}{dt} f(A_+ - t) \right)_{t=0} \eta(B) \\ &= if'(A_+)\eta(B). \end{aligned}$$

Therefore, the commutator  $Bf(A_+)\eta(B) - f(A_+)\eta(B)B$  extends to the bounded operator  $if'(A_+)\eta(B)$  by density of  $C_c^\infty(\mathbb{R}_+)$  in  $\mathcal{D}(B)$ . On another hand, if  $\mathcal{M} : L^2(\mathbb{R}_+) \rightarrow L^2(\mathbb{R})$  denotes the Mellin transform as given in [3, Sec. 1.5], then it is known that  $\mathcal{M}A_+\mathcal{M}^{-1} = X$  and  $\mathcal{M}B\mathcal{M}^{-1} = -P$ , with  $X$  the multiplication operator by the variable in  $L^2(\mathbb{R})$  and  $P$  the differentiation operator  $-i\nabla$  in  $L^2(\mathbb{R})$ . It follows that

$$f'(A_+)\eta(B) = \mathcal{M}^{-1}f'(X)\eta(-P)\mathcal{M},$$

with  $f'(X)\eta(-P)$  of trace class due to the decay assumption on  $f'$  (see [2, Cor. 4.1.4]). Therefore, the operator  $f'(A_+)\eta(B)$  is also trace class, and the second condition is verified. So, the relation (6.2) holds and implies that  $s\text{-}\lim_{t \rightarrow \pm\infty} e^{it e^{2B}} f(A_+) e^{-it e^{2B}} \varphi = f_{\mp} \varphi$  for each vector  $\varphi \in L^2(\mathbb{R}_+)$  such that  $\varphi = \eta(B)\varphi$  for some  $\eta \in C_c^\infty(\mathbb{R})$ . Since this set of vectors  $\varphi$  is dense in  $L^2(\mathbb{R}_+)$ , one infers that

$$s\text{-}\lim_{t \rightarrow \pm\infty} e^{it e^{2B}} f(A_+) e^{-it e^{2B}} = f_{\mp}.$$

Finally, using the fact that  $e^{2B} = \mathcal{F}_c(-\Delta_N)\mathcal{F}_c^{-1}$  and  $A_+ = -\mathcal{F}_c A_+ \mathcal{F}_c^{-1}$  with  $\mathcal{F}_c$  the cosine transform (2.2), one obtains from the last relation that

$$s\text{-}\lim_{t \rightarrow \pm\infty} e^{it(-\Delta_N)} f(-A_+) e^{-it(-\Delta_N)} = f_{\mp},$$

which is equivalent to (6.1). □

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