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Scattering through a straight quantum waveguide with combined boundary conditions

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Scattering through a straight two-dimensional quantum waveguide $\mathbb{R} \times (0, d)$ with Dirichlet boundary conditions on $(\mathbb{R}^*_- \times \{y = 0\}) \cup (\mathbb{R}^*_+ \times \{y = d\})$ and Neumann boundary condition on $(\mathbb{R}^*_- \times \{y = d\}) \cup (\mathbb{R}^*_+ \times \{y = 0\})$ is considered using stationary scattering theory. The existence of a matching conditions solution at $x = 0$ is proved. The use of stationary scattering theory is justified showing its relation to the wave packets motion. As an illustration, the matching conditions are also solved numerically and the transition probabilities are shown.

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I. INTRODUCTION

Free motion of the non-relativistic quantum mechanical particle is described by Laplace operator as the Hamiltonian up to unessential constants, i.e. if units where $\hbar = 1$ and particle mass $m = \frac{1}{2}$ are used. Impenetrable walls guiding the particle motion are described by boundary conditions on the wave function annulating the current through the walls and at the same time making the Laplacian to be a self-adjoint operator with the suitable domain. Restricting ourselves to the local boundary conditions, they are of the Robin form with the real coefficient. The important special cases are Dirichlet and Neumann boundary conditions known also from other parts of physics. They can also effectively appear for the wave functions of special symmetry, e.g.[1,2]. If walls with different types of boundary conditions can be realized e.g. in some semiconductor materials we would have at our disposal a new type of electron motion control giving perspectives of new microelectronic elements. The study of quantum mechanical problems with combined Dirichlet and Neumann boundary conditions is also a mathematical challenge which can lead to further solvable or nearly solvable models.

Two-dimensional straight quantum waveguides with the combined Dirichlet and Neumann boundary conditions are studied for years. They were examined as auxiliary problems in[1,2] and the existence of bound states was proved for some configurations. The existence of bound states in a Dirichlet planar waveguide with Neumann window was shown in[3]. In[4], the existence or non-existence of bound states for the cases of Dirichlet and Neumann boundary conditions on half-lines of each boundary were shown in dependence of the overlap of Neumann part projections to the waveguide axis. The Hamiltonian domain was also studied thoroughly. The existence of discrete spectrum for the same system was reconsidered also in[5] where a lower bound on the Hamiltonian of the Hardy inequality type was proved. Further details on the discrete spectrum were obtained in[6]. Paper[7] show the existence of bound states for the 3-dimensional layer with Dirichlet boundary conditions outside one or two Neumann disc-shaped windows. The time decay of heat equation solution in two-dimensional waveguides with combined boundary conditions was studied in[8]. The cases with infinitely many changes of boundary condition type were studied in[9]. The limit of infinitely thin waveguide was investigated in[10] and the Dirichlet-like decoupling of parts with different boundary conditions proved in the limit. In the above mentioned papers, mostly spectral

properties were studied.

In the present paper we investigate a simple situation of scattering occuring in the planar straight strip-like domain that is displayed on Figure **??**. The Hamiltonian H is the (minus) Laplace operator in the waveguide $\Omega = \mathbb{R} \times (0, d)$ with the Dirichlet boundary condition on $(\mathbb{R}^*_- \times \{0\}) \cup (\mathbb{R}^*_+ \times \{d\})$ and the Neumann boundary condition on $(\mathbb{R}^*_- \times \{d\}) \cup (\mathbb{R}^*_+ \times \{0\})$. Its domain reads (see[4])

$$\mathcal{D}(H) = \Big\{\psi \in H^1(\Omega) | -\Delta\psi \in L^2(\Omega), \\ \psi(-x,0) = \psi(x,d) = \frac{\partial\psi}{\partial y}(x,0) = \frac{\partial\psi}{\partial y}(-x,d) = 0 \text{ for } x > 0\Big\}.$$

The domain of H is not $H^2(\Omega)$ but it is contained in $H^2_{\mathrm{loc}}(\Omega)$. In fact, functions from $\mathcal{D}(H)$ are in $H^2(\Omega_1)$ for any open $\Omega_1 \subset \Omega$ such that $\overline{\Omega_1} \cap \{(0,0)\,,\,(0,d)\} = \emptyset$. This is an analogy of the well known situation for the Dirichlet Laplacian on a planar domains with angles larger than π on the boundary[11].

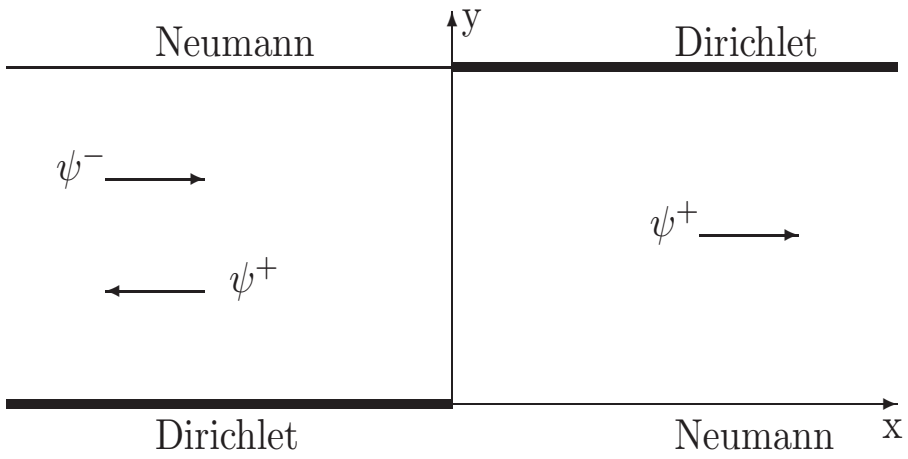

FIG. 1. The shape of waveguide.

We consider the scattering from the left ($x \to -\infty$) to the right ($x \to +\infty$), the oposite case being symmetric. As reference (free motion) Hamiltonians for the scattering we use two (minus) Laplace operators with Dirichlet boundary condition on the whole lower boundary $y = 0$ and Neumann boundary condition on the whole upper boundary $y = d$ or vice versa. Their spectral decompositions are clear from the variables separation. The corresponding

transversal modes are

$$\chi_n^-(y) = \sqrt{\frac{2}{d}} \sin\left((2n-1)\frac{\pi y}{2d}\right), \ \chi_n^+(y) = \sqrt{\frac{2}{d}} \cos\left((2n-1)\frac{\pi y}{2d}\right) \tag{1}$$

where $n \in \mathbb{N}^*$, with eigenvalues $\mu_n = (2n-1)^2 \frac{\pi^2}{4d^2}$.

We obtain the following results.

(i) There exists scattering stationary wave function $f(k,x,y)$ satisfying the stationary Schrödinger equation $(\Delta + E)f(k,x,y) = 0$ in the distributional sense inside the strip Ω, Dirichlet, respectively Neumann, boundary conditions at the appropriate parts of the boundary of Ω, and having the scattering asymtotics

$$f(k,x,y) \approx e^{ikx}\chi_{n_0}^-(y) + \sum_{l=1}^{n_1} r_l(k) e^{-ik_l x}\chi_l^-(y) \quad \text{as} \quad x \to -\infty \ ,$$

$$f(k,x,y) \approx \sum_{l=1}^{n_1} t_l(k) e^{ik_l x}\chi_l^+(y) \quad \text{as} \quad x \to +\infty \ .$$

Here $E > 0$ is the energy of scattered particle, $k > 0$ the longitudinal momentum of incoming particle, $k_l > 0$ outgoing momenta, $\chi_{n_0}^-$ incoming transversal mode, $\chi_l^\pm$ outgoing transversal modes, r_l and t_l reflection and transmission coefficients. The result is formulated below as Theorem 1, the proof consists of formulating the matching conditions at $x = 0$ and showing the existence of their solution.

(ii) From the non-integrable functions $f(k,\cdot,\cdot)$, time-dependent wave packets $\psi(t,\cdot,\cdot)$ are formed belonging to $L^2(\Omega)$ and the Hamiltonian domain and satisfying the time-dependent Schrödinger equation (Proposition 2). *Their scattering behavior is shown as asymptotics* (Theorem 3)

$$\lim_{t\to\pm\infty} \|\psi(t,\cdot,\cdot) - \psi^\pm(t,\cdot,\cdot)\|_{L^2(\Omega)} = 0$$

where $\psi^\pm$ are solutions of the free Schrödinger equations, i.e., ψ^- satisfies Dirichlet boundary condition at $y = 0$ and Neumann boundary condition at $y = d$ for arbitrary x, and vice versa for ψ^+.

II. STATIONARY SCATTERING WAVE FUNCTION

Given an initial transversal mode $n_0 \in \mathbb{N}^*$, we fix the energy $E \in (\mu_N, \mu_{N+1})$ for some natural number $N \geq n_0$ and pick a longitudinal momentum $k \in \mathbb{R}_+^*$ such that

$$E = \mu_{n_0} + k^2. \tag{2}$$

We skip the case of E equal to the energy of some transversal mode μ_n for some $n \in \mathbb{N}^*$, whose set has zero Lebesgue measure on the real line generated by k. Let us denote the maximal excitable transversal mode as

$$n_1(k) = \left[\frac{1}{2} + \sqrt{\left(n_0 - \frac{1}{2}\right)^2 + \frac{d^2}{\pi^2}k^2} \right], \tag{3}$$

where the symbol $[\cdot]$ stands for the integer part, and set

$$k_n = \sqrt{\mu_{n_0} - \mu_n + k^2} > 0, \text{ for } n = 1, 2, \ldots, n_1(k), \tag{4}$$

and

$$\kappa_n = \sqrt{\mu_n - \mu_{n_0} - k^2} > 0 \text{ for } n \geq n_1(k) + 1. \tag{5}$$

In light of (5) we may find constants $c_0(k), c_1(k) > 0$, depending only on k, such that the estimates

$$c_0(k) \leq \frac{\kappa_n(k)}{n} \leq c_1(k) \tag{6}$$

hold for all n sufficiently large.

We note $\mathcal{F}_{E,n_0,k}$ the set of functions $f(k,\cdot,\cdot)$ of the form

$$f(k,x,y) = e^{ikx}\chi_{n_0}^-(y) + \sum_{l=1}^{n_1} r_l(k)e^{-ik_l x}\chi_l^-(y) + \sum_{n=n_1+1}^{\infty} r_n(k)e^{\kappa_n x}\chi_n^-(y) \tag{7}$$

for $x < 0$, and

$$f(k,x,y) = \sum_{l=1}^{n_1} t_l(k)e^{ik_l x}\chi_l^+(y) + \sum_{n=n_1+1}^{\infty} t_n(k)e^{-\kappa_n x}\chi_n^+(y) \tag{8}$$

for $x > 0$. Here $r_n(k)$ and $t_n(k)$, for $n \in \mathbb{N}^*$, are complex coefficients.

We look for a function $f(k,\cdot,\cdot) \in \mathcal{F}_{E,n_0,k}$, which is solution to the eigenvalue equation $-\Delta f(k,\cdot,\cdot) = Ef(k,\cdot,\cdot)$ in Ω, and satisfies the following matching conditions

$$f(k,0^-,\cdot) = f(k,0^+,\cdot), \ \frac{\partial f}{\partial x}(k,0^-,\cdot) = \frac{\partial f}{\partial x}(k,0^+,\cdot). \tag{9}$$

We shall justify and precise (9) in subsection II B. We require in addition that $f(k,\cdot,\cdot)$ be locally in $\mathcal{D}(H)$, entailing that the restrictions of $f(k,\cdot,\cdot)$ to $(-L,0)\times(0,d)$ and $(0,L)\times(0,d)$ are respectively in $H^1((-L,0)\times(0,d))$ and $H^1((0,L)\times(0,d))$, for all $L > 0$. Namely, this yields that

$$\sum_{n=1}^{\infty} n|r_n|^2 < \infty \text{ and } \sum_{n=1}^{\infty} n|t_n|^2 < \infty. \tag{10}$$

A. Suitable functional spaces

For any $\alpha \in \mathbb{R}$, the space

$$\mathcal{H}^\alpha_\pm = \left\{ g = \sum_{n=1}^{\infty} c_n \chi_n^\pm \;\Big|\; \|g\|^2_{\alpha,\pm} = \sum_{n=1}^{\infty} n^{2\alpha} |c_n|^2 < \infty \right\}$$

is Hilbertian for the scalar product $(\cdot,\cdot)_{\alpha,\pm}$ induced by the above defined norm $\|\cdot\|_{\alpha,\pm}$. For $\alpha \geq 0$, $\mathcal{H}^\alpha_\pm \subset L^2(0,d)$ while for $\alpha < 0$ this is a space of functionals defined below. For all $f(k,\cdot,\cdot) \in \mathcal{F}_{E,n_0,k}$, it can be checked that the trace from left at $x = 0$,

$$f(k,0^-,y) = \chi^-_{n_0}(y) + \sum_{l=1}^{n_1} r_l(k)\chi^-_l(y) + \sum_{n=n_1+1}^{\infty} r_n(k)\chi^-_n(y), \tag{11}$$

belongs to $\mathcal{H}^{\frac{1}{2}}_-$, while the trace from right

$$f(k,0^+,y) = \sum_{n=1}^{\infty} t_n(k)\chi^+_n(y), \tag{12}$$

is in $\mathcal{H}^{\frac{1}{2}}_+$. Identity (11) (resp., (12)) may be verified upon taking finite partial sums in the right hand side of (7) (resp., (8)) as approximating C^∞-functions in $H^1((-L,0)\times(0,d))$ norm (resp., $H^1((0,L)\times(0,d))$ norm) and combining the exponential decay of the corresponding terms for $x \neq 0$ with (10).

Imposing on $f(k,\cdot,\cdot)$ that the two expressions in the right hand side of (11) and (12) coincide in $L^2(0,d)$, the common value $f(k,0^-,\cdot) = f(k,0^+,\cdot)$ then belongs to the space $\mathcal{H}^{\frac{1}{2}} = \mathcal{H}^{\frac{1}{2}}_- \cap \mathcal{H}^{\frac{1}{2}}_+$. More generally, for any $\alpha > 0$, the space $\mathcal{H}^\alpha = \mathcal{H}^\alpha_- \cap \mathcal{H}^\alpha_+$, endowed with the scalar product, $(f,g)_\alpha = (f,g)_{\alpha,-} + (f,g)_{\alpha,+}$, is Hilbertian and thus a reflexive Banach space. Moreover, the dual space $(\mathcal{H}^\alpha_\pm)'$ of $\mathcal{H}^\alpha_\pm$, and $\mathcal{H}^{-\alpha}_\pm$ are isometric. These two spaces may be identified through the duality bracket

$$(f,g)_{\mathcal{H}^{-\alpha}_\pm,\mathcal{H}^\alpha_\pm} = \sum_{n=1}^{+\infty} \overline{f_n} g_n, \;\; f = \sum_{n=1}^{+\infty} f_n \chi^\pm_n, \;\; g = \sum_{n=1}^{+\infty} g_n \chi^\pm_n.$$

Analogously, we put for every $\alpha > 0$,

$$\mathcal{H}^{-\alpha} = (\mathcal{H}^\alpha)' \supset \mathcal{H}^{-\alpha}_- \cup \mathcal{H}^{-\alpha}_+,$$

and we write $(f,g)_{-\alpha,\alpha}$ instead of $(f,g)_{\mathcal{H}^{-\alpha},\mathcal{H}^\alpha}$.

B. Matching conditions

As we seek for generalized eigenfunctions of the operator H, we look for the solution f to the equation $(\Delta + E)f = 0$ in Ω, where $E \in \mathbb{R}$.

For $k \in \mathbb{R}$ fixed, we know from (6) that κ_n scales like n so the series appearing in (7) (resp., in (8)) converges locally uniformly in $(-\infty, 0) \times (0, d)$ (resp., on $(0, +\infty) \times (0, d)$). Differentiating term by term in (7)-(8) we obtain through direct computation that any function $f(k, \cdot, \cdot) \in \mathcal{F}_{E,n_0,k}$ verifies $(\Delta + E)f(k, x, y) = 0$ for every $(x, y) \in \mathbb{R}^*_\pm \times (0, d)$ pointwise as well as distributionally. For every $\varphi \in C_0^\infty(\Omega)$, it follows from this upon applying Stokes theorem that the scalar product $(f(k, \cdot, \cdot), (\Delta + E)\varphi)_{L^2(\Omega)}$ expresses as:

$$\lim_{\varepsilon \downarrow 0} \left(\int_0^d \bar{f}(k, -\varepsilon, y) \frac{\partial \varphi}{\partial x}(-\varepsilon, y) dy - \int_0^d \bar{f}(k, \varepsilon, y) \frac{\partial \varphi}{\partial x}(\varepsilon, y) dy \right.$$
$$\left. - \int_0^d \frac{\partial \bar{f}}{\partial x}(k, -\varepsilon, y) \varphi(-\varepsilon, y) dy + \int_0^d \frac{\partial \bar{f}}{\partial x}(k, \varepsilon, y) \varphi(\varepsilon, y) dy \right). \tag{13}$$

Taking the limit in the above identity and bearing in mind that $f(k, 0^\pm, \cdot) \in \mathcal{H}^{\frac{1}{2}}_\pm \subset L^2(0, d)$, we find out that

$$\begin{aligned} &(f(k, \cdot, \cdot), (\Delta + E)\varphi)_{L^2(\Omega)} \\ &= \left(f(k, 0^-, \cdot) - f(k, 0^+, \cdot), \frac{\partial \varphi}{\partial x}(0, \cdot) \right)_{L^2(0,d)} \\ &\quad + (f_x(k, 0^+, \cdot) - f_x(k, 0^-, \cdot), \varphi(0, \cdot))_{-\frac{1}{2}, \frac{1}{2}}, \end{aligned} \tag{14}$$

for all $\varphi \in C_0^\infty(\Omega)$. Here $\varphi(0, \cdot)$ is regarded as an element of $\mathcal{H}^{\frac{1}{2}}$, and

$$f_x(k, 0^-, \cdot) = ik\chi^-_{n_0} - i \sum_{l=1}^{n_1} k_l r_l(k) \chi^-_l + \sum_{n=n_1+1}^{\infty} \kappa_n r_n(k) \chi^-_n \in \mathcal{H}^{-\frac{1}{2}}_-, \tag{15}$$

$$f_x(k, 0^+, \cdot) = i \sum_{l=1}^{n_1} k_l t_l(k) \chi^+_l - \sum_{n=n_1+1}^{\infty} \kappa_n t_n(k) \chi^+_n \in \mathcal{H}^{-\frac{1}{2}}_+. \tag{16}$$

The two above expressions are obtained upon formally differentiating at $x = 0$ each term in the series (7)-(8) with respect to x. Actually, (15)-(16) may be rigorously justified with the help of (5) and (10). We refer to Appendix B for more details. In light of (14) we have obtained the following result.

Proposition 1 *For $n_0 \in \mathbb{N}^*$ fixed, pick $E \in (\mu_{n_0}, \infty)$ and $k \in \mathbb{R}^*_+$ in accordance with (2) and let $f(k, \cdot, \cdot) \in \mathcal{F}_{E,n_0,k}$. Assume moreover that the two following conditions holds*

simultaneously:

$$f(k,0^-,\cdot) = f(k,0^+,\cdot) \quad \text{in } \mathcal{H}^{\frac{1}{2}} \tag{17}$$

$$f_x(k,0^-,\cdot) = f_x(k,0^+,\cdot) \quad \text{in } \mathcal{H}^{-\frac{1}{2}} \tag{18}$$

where $f_x(k,0^\pm,\cdot)$ is defined in (15)-(16). Then we have $(\Delta+E)f(k,\cdot,\cdot)=0$ in the distributional sense in Ω.

Remark 1 *The equality (17) is a necessary condition for the conclusion of Proposition 1 to hold, but we do not know whether this is the case for (18). This can be seen upon taking $\varphi(x,y)=\varphi_1(x)\varphi_2(y)$ in (14) for two arbitrary functions $\varphi_1 \in C_0^\infty(\mathbb{R})$ and $\varphi_2 \in C_0^\infty(0,d)$, getting that both terms in the right hand side of (14) vanish. This entails that $f(k,0^-,\cdot)=f(k,0^+,\cdot)$ in $L^2(0,d)$, which yields (17), and that the restrictions of $f_x(k,0^-,\cdot)$ and $f_x(k,0^+,\cdot)$ to $C_0^\infty(0,d)$ coincide. As we did not succeed to prove that $C_0^\infty(0,d)$ is dense in $\mathcal{H}^{\frac{1}{2}}$, it is not clear whether (18) can be derived from this. Notice that it is not clear whether our $\mathcal{H}^{\frac{1}{2}} = \mathcal{H}_-^{\frac{1}{2}} \cap \mathcal{H}_+^{\frac{1}{2}}$ given as intersection with the above defined norm is the standard Sobolev space $H_0^{\frac{1}{2}}$.*

C. Existence result

This section is devoted to proving the existence of an actual $f(k,\cdot,\cdot) \in \mathcal{F}_{E,n_0,k}$ satisfying the stationary Schrödinger equation $(\Delta+E)f=0$ in the distributional sense in Ω. In light of Proposition 1, it is enough to seek for a function $f(k,\cdot,\cdot)$ in $\mathcal{F}_{E,n_0,k}$ fulfilling the matching conditions (17)-(18). With reference to (17), we denote by $\varphi = f(k,0^-,\cdot) = f(k,0^+,\cdot)$ the common value in $\mathcal{H}^{\frac{1}{2}}$ of traces from left and right at $x=0$ of $f(k,\cdot,\cdot)$. In view of (7)-(8), we have

$$\varphi = \chi_{n_0}^- + \sum_{n=1}^{\infty} r_n(k)\chi_n^- = \sum_{n=1}^{\infty} t_n(k)\chi_n^+ \in \mathcal{H}^{\frac{1}{2}}. \tag{19}$$

Relation (19) holds necessarily in $L^2(0,d)$, expressing the function φ in two different Hilbertian basis of this space, so there is one-to-one correspondence between the coefficients $r_n(k)$ and $t_n(k)$. We are thus left with the task of finding a function φ of the form prescribed by (19) which fulfills (18). To this purpose we put for all $n \in \mathbb{N}^*$,

$$p_n^\pm = (\chi_n^\pm,\cdot)_{L^2(0,d)}\chi_n^\pm, \tag{20}$$

and we recall (15)-(16) and (19) in order to re-express $f_x(k,0^\pm,\cdot)$ in terms of φ, getting:

$$f_x(k,0^-,\cdot) = \left(-i\sum_{l=1}^{n_1} k_l p_l^- + \sum_{n=n_1+1}^{\infty} \kappa_n p_n^-\right)\varphi + 2ik\chi_{n_0}^-,$$
$$f_x(k,0^+,\cdot) = \left(i\sum_{l=1}^{n_1} k_l p_l^+ - \sum_{n=n_1+1}^{\infty} \kappa_n p_n^+\right)\varphi.$$

In light of the two above identities, the matching condition (18) may be equivalently reformulated as

$$D\varphi = -2ik\chi_{n_0}^-, \tag{21}$$

where $D : \mathcal{H}^{\frac{1}{2}} \to \mathcal{H}^{-\frac{1}{2}}$ is the operator

$$D = -iD_1 + D_2,\ D_1 = \sum_{l=1}^{n_1} k_l(p_l^- + p_l^+),\ D_2 = \sum_{n=n_1+1}^{\infty} \kappa_n(p_n^- + p_n^+). \tag{22}$$

Since k_n/n and κ_n/n are both majorized by $2\sqrt{E}$, uniformly in $n \in \mathbb{N}^*$, then the estimate

$$\|D\psi\|_{-\frac{1}{2}} \leq 2\sqrt{E}\|\psi\|_{\frac{1}{2}}$$

holds true for any $\psi = \sum_{n\geq 1} a_n\chi_n^- = \sum_{n\geq 1} b_n\chi_n^+ \in \mathcal{H}^{\frac{1}{2}}$. As a consequence, the linear operator D is bounded from $\mathcal{H}^{\frac{1}{2}}$ into $\mathcal{H}^{-\frac{1}{2}}$, with $\|D\|_{\mathcal{B}(\mathcal{H}^{\frac{1}{2}},\mathcal{H}^{-\frac{1}{2}})} \leq 2\sqrt{E}$.

The proof of the existence of φ obeying (21) boils down to the following technical but essential result, whose proof is postponed to Appendix A 2.

Lemma 1 *The operator D_2 is a strictly positive and boundedly invertible from $\mathcal{H}^{\frac{1}{2}}$ onto $\mathcal{H}^{-\frac{1}{2}}$. Moreover, the restriction $(D_2^{-1})_{|L^2(0,d)}$ of D_2^{-1} to $L^2(0,d)$, is symmetric.*

In light of (22), the matching condition (21) reads $-iD_1\varphi + D_2\varphi = -2ik\chi_{n_0}^-$ so it may be equivalently rephrased as

$$\varphi - iD_2^{-1}D_1\varphi = -2ikD_2^{-1}\chi_{n_0}^-, \tag{23}$$

according to Lemma 1.

For every $n \in \mathbb{N}^*$, we denote by P_n the orthogonal projection onto the finite dimensional subspace $\mathcal{P}_n = \mathrm{span}\{\chi_j^\pm,\ j = 1,\dots,n\}$. Due to (4), D_1 is a positive self-adjoint bounded operator in $\mathcal{P}_{n_1}$ and the same is true for $D_1^{1/2}$ and its inverse $D_1^{-1/2}$. Further, putting

$$\varphi_1 = D_1^{1/2}P_{n_1}\varphi,$$

we may rewrite (23) as $\varphi - iD_2^{-1}D_1^{1/2}\varphi_1 = -2ikD_2^{-1}\chi_{n_0}^-$. Applying $D_1^{1/2}P_{n_1}$ and $I - P_{n_1}$ successively to both sides of the above equation, we end up getting that (23) is equivalent to the system formed by the two following equations:

$$(I - iD_1^{1/2}P_{n_1}D_2^{-1}P_{n_1}D_1^{1/2})\varphi_1 = -2ikD_1^{1/2}P_{n_1}D_2^{-1}\chi_{n_0}^- \tag{24}$$

$$\varphi_2 - i(I - P_{n_1})D_2^{-1}P_{n_1}D_1^{1/2}\varphi_1 = -2ik(I - P_{n_1})D_2^{-1}\chi_{n_0}^-, \tag{25}$$

where

$$\varphi_2 = (I - P_{n_1})\varphi.$$

Notice from the second part of Lemma 1 that the operator $M = D_1^{1/2}P_{n_1}D_2^{-1}P_{n_1}D_1^{1/2}$ is symmetric in $\mathcal{P}_{n_1}$. As a consequence, all the eigenvalues λ_j, $j = 1, \ldots, n_1$, of M, are real and $\det(I - iM) = \prod_{j=1}^{n_1}(1 - i\lambda_j) \neq 0$, showing that (24) admits a unique solution $\varphi_1 \in \mathcal{P}_{n_1} \subset L^2(0, d)$. From this and (25) then follows that $\varphi_2 \in L^2(0, d)$, which in turn yields

$$\varphi = D_1^{-\frac{1}{2}}\varphi_1 + \varphi_2 = iD_2^{-1}(P_{n_1}D_1^{1/2}\varphi_1 - 2k\chi_{n_0}^-) \in \mathcal{H}^{\frac{1}{2}},$$

since $L^2(0, d) \subset \mathcal{H}^{-\frac{1}{2}}$. This proves the existence of φ and consequently of f. Summing up, we have obtained the:

Theorem 1 *Let n_0, E and k be the same as in Proposition 1. Then there exists $f(k, \cdot, \cdot) \in \mathcal{F}_{E,n_0,k}$ satisfying the equation $(\Delta + E)f(k, \cdot, \cdot) = 0$ in the distributional sense in Ω.*

Remark 2 *Let $\psi \in \mathcal{H}^{-\frac{1}{2}}$ be arbitrary. It is clear that the above reasonning remains valid upon substituting ψ for $-2ik\chi_{n_0}^-$ in the right hand side of (21). Therefore the equation $D\varphi = \psi$ admits a unique solution solution $\varphi \in \mathcal{H}^{\frac{1}{2}}$. This entails that the linear bounded operator D is invertible from $\mathcal{H}^{\frac{1}{2}}$ onto $\mathcal{H}^{-\frac{1}{2}}$. By the inverse mapping theorem, its inverse D^{-1} is thus bounded from $\mathcal{H}^{-\frac{1}{2}}$ onto $\mathcal{H}^{\frac{1}{2}}$.*

D. Smooth k-dependence

For all $(x, y) \in \mathbb{R}^* \times (0, d)$, it is apparent from (7)-(8) that $k \mapsto f(k, x, y)$ is continuously differentiable in $\mathbb{R} \setminus M$, where the set

$$M = \{k \in \mathbb{R}_+^* \,|\, \exists n \in \mathbb{N}^*,\ \mu_n = k^2 + \mu_{n_0}\}$$

is discrete. Moreover, for $x = 0$ we have the:

Theorem 2 *The solution to (21), regarded as a function of the parameter $k \in \mathbb{R}_+^*$, belongs to $C^1(\mathbb{R}_+^* \setminus M; \mathcal{H}^{\frac{1}{2}})$.*

Proof. We prove that $k \mapsto f(k, 0, y)$ is continuously differentiable for any $y \in (0, d)$. To this purpose we first estimate the variation of the operators $D = D(k)$ with respect to k. To do that we fix $k \in \mathbb{R}$ and refer to (4)-(5) in order to choose $\varepsilon_1 = \varepsilon_1(k) > 0$ so small that $n_1(k+\varepsilon) = n_1(k)$ for $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$. Then we apply (22), getting

$$\begin{aligned} D(k+\varepsilon) - D(k) = -i \sum_{l=1}^{n_1} (k_l(k+\varepsilon) - k_l(k))(p_l^- + p_l^+) \\ + \sum_{n=n_1+1}^{\infty} (\kappa_n(k+\varepsilon) - \kappa_n(k))(p_n^- + p_n^+), \end{aligned} \tag{26}$$

where n_1 stands for $n_1(k) = n_1(k+\varepsilon)$. Next we recall from (4)-(5) that there exist a continuous functions $c_n(k, \cdot)$ obeying

$$\begin{aligned} k_n(k+\varepsilon) - k_n(k) &= \frac{k}{k_n(k)}\varepsilon + c_n(k,\varepsilon)\varepsilon^2, \ n = 1, .., n_1, \\ \kappa_n(k+\varepsilon) - \kappa_n(k) &= -\frac{k}{\kappa_n(k)}\varepsilon + c_n(k,\varepsilon)\varepsilon^2, \ n \geq n_1 + 1, \end{aligned}$$

for $(-\varepsilon_1, \varepsilon_1)$. Moreover, we know from (6) that the estimate $|c_n(k,\varepsilon)| \leq c(k)/n$ holds uniformly in $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$, where the constant $c(k) > 0$ depends only on k and ε_1. Hence

$$C(k,\varepsilon) = \sum_{n=1}^{\infty} c_n(k,\varepsilon)(p_n^- + p_n^+) \in \mathcal{B}(\mathcal{H}^{\frac{1}{2}}, \mathcal{H}^{-\frac{1}{2}}),$$

with

$$\|C(k,\varepsilon)\|_{\mathcal{B}(\mathcal{H}^{\frac{1}{2}}, \mathcal{H}^{-\frac{1}{2}})} \leq c(k), \ \varepsilon \in (-\varepsilon_1, \varepsilon_1). \tag{27}$$

for some positive constant $c(k)$ independent of ε. Arguing in the same way as above we obtain that the linear term with respect to ε, appearing in (26), satisfies

$$\left\| -ik \sum_{l=1}^{n_1} \frac{1}{k_l}(p_l^- + p_l^+) - k \sum_{n=n_1+1}^{\infty} \frac{1}{\kappa_n}(p_n^- + p_n^+) \right\|_{\mathcal{B}(\mathcal{H}^{\frac{1}{2}}, \mathcal{H}^{-\frac{1}{2}})} \leq c(k), \tag{28}$$

where $c(k)$ is another constant depending only on k. Putting (26) and (27)-(28) together we obtain for all $|\varepsilon| < \varepsilon_1$ that

$$\|D(k+\varepsilon) - D(k)\|_{\mathcal{B}(\mathcal{H}^{\frac{1}{2}}, \mathcal{H}^{-\frac{1}{2}})} \leq c(k)\varepsilon(1+\varepsilon),$$

hence $\|D(k)^{-1}(D(k+\varepsilon) - D(k))\|_{\mathcal{B}(\mathcal{H}^{\frac{1}{2}})} < 1$, upon eventually shortening ε_1. Therefore $I + D(k)^{-1}(D(k+\varepsilon) - D(k))$ is invertible in $\mathcal{B}(\mathcal{H}^{\frac{1}{2}})$ for every $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$ and the same

is true for $D(k+\varepsilon) = D(k)(I + D(k)^{-1}(D(k+\varepsilon) - D(k)))$ in $\mathcal{B}(\mathcal{H}^{\frac{1}{2}}, \mathcal{H}^{-\frac{1}{2}})$. Moreover $\|D(k+\varepsilon)^{-1}\|_{\mathcal{B}(\mathcal{H}^{-\frac{1}{2}},\mathcal{H}^{\frac{1}{2}})}$ is uniformly bounded by, say, $c' = c'(k) > 0$, in $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$. Thus, bearing in mind that

$$\begin{aligned}
&\|D(k+\varepsilon)^{-1} - D(k)^{-1}\|_{\mathcal{B}(\mathcal{H}^{-\frac{1}{2}},\mathcal{H}^{\frac{1}{2}})} \\
&= \|D(k)^{-1}(D(k) - D(k+\varepsilon))D(k+\varepsilon)^{-1}\|_{\mathcal{B}(\mathcal{H}^{-\frac{1}{2}},\mathcal{H}^{\frac{1}{2}})} \\
&\leq c'^2 \|(D(k) - D(k+\varepsilon))\|_{\mathcal{B}(\mathcal{H}^{\frac{1}{2}},\mathcal{H}^{-\frac{1}{2}})},
\end{aligned}$$

we end up getting that

$$\lim_{\varepsilon \to 0} \|D(k+\varepsilon)^{-1} - D(k)^{-1}\|_{\mathcal{B}(\mathcal{H}^{-\frac{1}{2}},\mathcal{H}^{\frac{1}{2}})} = 0. \tag{29}$$

For $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$, let $\varphi(k+\varepsilon) = D(k+\varepsilon)^{-1}(-2i(k+\varepsilon)\chi_{n_0}^-)$ denotes the solution to (21). Then we have $D(k+\varepsilon)(\varphi(k+\varepsilon) - \varphi(k)) = -(D(k+\varepsilon) - D(k))\varphi(k) - 2i\varepsilon\chi_{n_0}^-$ by direct calculation, hence

$$\begin{aligned}
&\frac{\varphi(k+\varepsilon) - \varphi(k)}{\varepsilon} \\
&= -D(k+\varepsilon)^{-1}\partial_k D(k)\varphi(k) - 2iD(k+\varepsilon)^{-1}\chi_{n_0}^- - \varepsilon D(k+\varepsilon)^{-1}C(k,\varepsilon)\varphi(k),
\end{aligned}$$

for any $0 < |\varepsilon| < \varepsilon_1$, where

$$\partial_k D(k) = -ik\sum_{l=1}^{n_1} \frac{1}{k_l}(p_l^- + p_l^+) - k\sum_{n=n_1+1}^{\infty} \frac{1}{\kappa_n}(p_n^- + p_n^+).$$

From this, (27) and (29) then follows that φ is differentiable in $\mathcal{H}^{\frac{1}{2}}$ at k, with

$$\frac{\partial\varphi}{\partial k}(k) = -D(k)^{-1}\partial_k D(k)\varphi(k) - 2iD(k)^{-1}\chi_{n_0}^- \in \mathcal{H}^{\frac{1}{2}}.$$

Notice that this expression coincides with the one obtained by formal differentiation of (21). Its continuity with respect to k was actually established in the proof.

□

Remark 3 *By induction, the continuity for higher derivatives of $k \mapsto \varphi(k)$ follows from the reasoning developped in the proof of Theorem 2.*

III. TIME-DEPENDENT SOLUTIONS

We now characterize the scattering properties of the physical model under study with the aid of the generalized eigenfunctions of H, described in section II (see Theorem 1). For the sake of simplicity we consider sufficiently small quasi-momenta intervals $[\alpha, \beta]$, with $0 < \alpha < \beta$, so that the index $n_1(k)$ of the highest excited transversal mode remains constant with respect to $k \in [\alpha, \beta]$. For any fixed $k_0 \in \mathbb{R}$, it is clear from (3) that this can be achieved upon imposing

$$\sqrt{\mu_{n_1(k_0)} - \mu_{n_0}} < \alpha < \beta < \sqrt{\mu_{n_1(k_0)+1} - \mu_{n_0}}. \tag{30}$$

Let $a \in C_0^\infty(\mathbb{R})$ be such that

$$\text{supp } a \subset [\alpha, \beta] \subset (0, \infty) \setminus M, \tag{31}$$

where M is as in Theorem 2, and let $f \in \mathcal{F}_{E,n_0,k}$ be defined by Theorem 1. In view of characterizing the asymptotic behaviour of the time-evolution generated by H of

$$\psi(t, x, y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} f(k, x, y) dk, \tag{32}$$

we introduce the two following states,

$$\psi^-(t, x, y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} e^{ikx} \chi_{n_0}^-(y)\, dk \tag{33}$$

and

$$\psi^+(t, x, y) = \begin{cases} \psi_{DN}(t, x, y) & \text{if } x < 0, \\ \psi_{ND}(t, x, y) & \text{if } x > 0, \end{cases} \tag{34}$$

where we have set

$$\psi_{DN}(t, x, y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} \sum_{l=1}^{n_1} r_l(k) e^{-ik_l x} \chi_l^-(y) dk, \tag{35}$$

$$\psi_{ND}(t, x, y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} \sum_{l=1}^{n_1} t_l(k) e^{ik_l x} \chi_l^+(y) dk. \tag{36}$$

As can be seen from the following statement, ψ_{DN} (resp. ψ_{ND}) is a weak solution to the Schrödinger equation associated with the Laplace operator Δ_{DN} (resp. Δ_{ND}) acting in $L^2(\Omega)$ with the Dirichlet (resp. Neumann) boundary conditions at $y = 0$ and Neumann (resp. Dirichlet) boundary conditions at $y = d$.

Proposition 2 *For every $t \in \mathbb{R}$, the function $\psi(t,\cdot,\cdot)$, defined by (32), belongs to $\mathcal{D}(H)$. Moreover ψ is a solution to the equation*

$$\left(i\frac{\partial}{\partial t} + H\right)\psi = 0. \tag{37}$$

Similarly $\psi^-(t,\cdot,\cdot) \in \mathcal{D}(\Delta_{DN})$ for each $t \in \mathbb{R}$ and we have

$$\left(i\frac{\partial}{\partial t} + \Delta_{DN}\right)\psi^- = 0. \tag{38}$$

Finally $\psi_{DN}(t,\cdot,\cdot)$ and $\psi_{ND}(t,\cdot,\cdot)$ are respectively in $\mathcal{D}(\Delta_{DN})$ and in $\mathcal{D}(\Delta_{ND})$ for all $t \in \mathbb{R}$, with

$$\left(i\frac{\partial}{\partial t} + \Delta_{DN}\right)\psi_{DN} = \left(i\frac{\partial}{\partial t} + \Delta_{ND}\right)\psi_{ND} = 0. \tag{39}$$

Proof. We only show the first part of the statement, the remaining part being obtained by arguing in the same way.

From the expression (19) of $\varphi = f(k,0^-,\cdot) = f(k,0^+,\cdot)$ we get that $r_n(k) = (\chi_n^-(\cdot),\varphi(k,\cdot))_{L^2(0,d)}$ (up to some additive constant for $n = n_0$) and $t_n(k) = (\chi_n^+(\cdot),\varphi(k,\cdot))_{L^2(0,d)}$ for any $n \in \mathbb{N}^*$. Each r_n and t_n as well as $\|\varphi\|_{\frac{1}{2}}$ is thus a continuous function of $k \in [\alpha,\beta]$ by Theorem 2. Therefore there exists a constant $c_1 > 0$ such that we have

$$|r_n(k)| \le c_1 n^{-\frac{1}{2}} \quad \text{and} \quad |t_n(k)| \le c_1 n^{-\frac{1}{2}}, \tag{40}$$

for all $n \ge 1$ and $k \in [\alpha,\beta]$, by (10). On the other hand (5) yields $\kappa_n \ge c_2 n$ uniformly in $n \ge n_1 + 1$ and $k \in [\alpha,\beta]$, for another positive constant c_2. As a consequence the function defined by

$$\tilde{\psi}_{ND}(t,x,y) = \int_{\mathbb{R}} a(k)e^{-i(\mu_{n_0}+k^2)t} \sum_{n=n_1+1}^{\infty} t_n(k)e^{-\kappa_n x}\chi_n^+(y)dk, \tag{41}$$

for every $(t,x,y) \in \mathbb{R} \times \mathbb{R}_+^* \times (0,d)$, satisfies

$$\begin{aligned}\int_0^d |\tilde{\psi}_{ND}(t,x,y)|^2 dy &= \sum_{n=n_1+1}^{\infty} \left|\int_{\mathbb{R}} a(k)e^{-i(\mu_{n_0}+k^2)t}t_n(k)e^{-\kappa_n x}\,dk\right|^2 \\ &\le c_1^2\|a\|_{L^1(\mathbb{R})}^2 \sum_{n=n_1+1}^{\infty} \frac{e^{-2c_2 nx}}{n}, \qquad (t,x) \in \mathbb{R} \times \mathbb{R}_+^*,\end{aligned}$$

whence

$$\int_0^\infty \int_0^d |\tilde{\psi}_{ND}(t,x,y)|^2 dydx \le \frac{c_1^2\|a\|_{L^1(\mathbb{R})}^2}{2c_2}\left(\sum_{n=n_1+1}^{\infty}\frac{1}{n^2}\right) < \infty.$$

Therefore $\tilde{\psi}_{ND}(t,\cdot,\cdot) \in L^2(\mathbb{R}_+^* \times (0,d))$ for any $t \in \mathbb{R}$, and we get in the same way that $\tilde{\psi}_{DN}(t,\cdot,\cdot) \in L^2(\mathbb{R}_-^* \times (0,d))$, where we have set

$$\tilde{\psi}_{DN}(t,x,y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} \sum_{n=n_1+1}^{\infty} r_n(k) e^{\kappa_n x} \chi_n^-(y) dk, \tag{42}$$

for all $(t,x,y) \in \mathbb{R} \times \mathbb{R}_-^* \times (0,d)$. By performing the change of integration variable $k \to k_l$ in each term of the sum appearing in (35)-(36), we obtain the Fourier transform of an L^2-function (with respect to the variable k_l), which is consequently square integrable with respect to x. Therefore the functions defined in (35)-(36) are lying in $L^2(\Omega)$, and we have $\psi \in L^2(\Omega)$ from (7)-(8) and (32).

The next step of the proof is to check out that the first order partial derivatives of $\psi(t,\cdot,\cdot)$ are square integrable in Ω for any $t \in \mathbb{R}$. We shall do it for $\partial\psi/\partial y$, the case of $\partial\psi/\partial x$ being handled in the same manner. We start by computing $\partial\psi/\partial y$ in the distributional sense. We have

$$\begin{aligned} &\langle \frac{\partial \psi}{\partial y}(t,\cdot,\cdot), \zeta \rangle_{(C_0^\infty(\Omega))', C_0^\infty(\Omega)} \\ &= -\int_\Omega \left(\int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} f(k,x,y) dk \right) \frac{\partial \zeta}{\partial y}(x,y) dx dy, \end{aligned} \tag{43}$$

for any arbitrary test function $\zeta \in C_0^\infty(\Omega)$. For $y \in (0,d)$ and $k \in \mathbb{R}$ fixed, we deduce from (8) that $|f(k,x,y)|$ is majorized by

$$\begin{aligned} &\left(\frac{2}{d}\right)^{1/2} \left(\sum_{l=1}^{n_1} |t_l(k)| + \sum_{n=n_1+1}^{\infty} |t_n(k)| e^{-c_2 n x} \right) \\ &\leq \left(\frac{2}{d}\right)^{1/2} \left(\sum_{l=1}^{n_1} |t_l(k)| + (1-e^{-2c_2 x})^{-\frac{1}{2}} \left(\sum_{n=n_1+1}^{\infty} |t_n(k)|^2 \right)^{1/2} \right), \end{aligned}$$

for all $x > 0$, and a similar estimate holds from (7) for $x < 0$. Hence the integral over (supp ζ) $\times$ (supp a) in the right hand side of (43) converges so we may apply Fubini's theorem. By integrating by parts over y, we find out by direct calculation that

$$\frac{\partial \psi}{\partial y}(t,x,y) = \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} f_y(k,x,y) dk,$$

in the distributional sense, where $f_y(k,x,y)$ expresses as

$$\mu_{n_0}^{1/2} e^{ikx} \chi_{n_0}^+(y) + \sum_{l=1}^{n_1} \mu_l^{1/2} r_l(k) e^{-ik_l x} \chi_l^+(y) + \sum_{n=n_1+1}^{\infty} \mu_n^{1/2} r_n(k) e^{\kappa_n x} \chi_n^+(y),$$

for $x < 0$, and as

$$-\left(\sum_{l=1}^{n_1} \mu_l^{1/2} t_l(k) e^{ik_l x} \chi_l^-(y) + \sum_{n=n_1+1}^{\infty} \mu_n^{1/2} t_n(k) e^{-\kappa_n x} \chi_n^-(y)\right),$$

for $x > 0$. We are thus left with the task of checking out that the two above expressions lead to square integrable functions in Ω. Since this is obviously the case for all terms expressed by a finite sum, we shall only examine the one of

$$\hat{\psi}_{ND}(t,x,y) = \sum_{n=n_1+1}^{\infty} \mu_n^{1/2} \chi_n^-(y) \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} t_n(k) e^{-\kappa_n x} dk.$$

Actually, it turns out that

$$\int_0^d \left|\hat{\psi}_{ND}(t,x,y)\right|^2 dy = \sum_{n=n_1+1}^{\infty} \mu_n \left|\int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} t_n(k) e^{-\kappa_n x}\, dk\right|^2$$

so we have

$$\begin{aligned} &\int_0^\infty \int_0^d \left|\hat{\psi}_{ND}(t,x,y)\right|^2 dxdy \\ &\leq \|a\|^2_{L^2(\mathbb{R})} \int_{\operatorname{supp} a} \sum_{n=n_1+1}^{\infty} \frac{\mu_n}{2\kappa_n(k)} |t_n(k)|^2 dk < \infty, \end{aligned}$$

the last series being majorized (up to some multiplicative constant) by $\|\varphi(k)\|^2_{\frac{1}{2}}$, which is bounded on $\operatorname{supp} a$. Now, bearing in mind that $f(k,\cdot,\cdot)$ is locally in the domain of the Laplacian (this is guaranteed by the matching conditions (17)-(18)), so that $x \mapsto f(k,\cdot,y) \in C^1(\mathbb{R})$ for almost every $y \in (0,d)$ and any arbitrary fixed k, we may apply the same method to $\partial\psi/\partial x$, proving that $\psi(t,\cdot,\cdot) \in H^1(\Omega)$.

Further, as ψ evidently satisfies the specified boundary conditions, it remains to prove (37), which involves calculating $\Delta\psi$ in the distributional sense. Arguing as above, we find out that,

$$-\Delta\psi(t,x,y) = \int_{\mathbb{R}} (\mu_{n_0} + k^2) a(k) e^{-i(\mu_{n_0}+k^2)t} f(k,x,y) dk, \tag{44}$$

with the integrand lying in $L^2(\Omega)$. Since the r.h.s. of (44) coincides with $-i\partial\psi(t,x,y)/\partial t$ (the derivative is computed for the topology of the norm in $L^2(\Omega)$), we end up getting (37).

□

Having established the main properties of the functions ψ defined by (32) and $\psi^\pm$ defined by (33)–(36) in Proposition 2, we are in position to prove the main result of this section.

Theorem 3 *Let $a \in C_0^1(\mathbb{R})$ obey* (30)-(31)*, let ψ be the same as in* (32) *and let $\psi^{\pm}$ be defined by* (33)–(36)*. Then we have*

$$\lim_{t\to\pm\infty} \|\psi(t,\cdot,\cdot) - \psi^{\pm}(t,\cdot,\cdot)\|_{L^2(\Omega)} = 0. \tag{45}$$

Proof. We first examine the case of $t > 0$. In light of (7)-(8), (32)–(36) and (41)-(42), the function ψ decomposes for any $x \in \mathbb{R}$ as

$$\begin{aligned}\psi(\cdot,x,\cdot) = \theta(-x)&\left(\psi^-(\cdot,x,\cdot) + \psi_{DN}(\cdot,x,\cdot) + \tilde{\psi}_{DN}(\cdot,x,\cdot)\right)\\ &+ \theta(x)\left(\psi_{ND}(\cdot,x,\cdot) + \tilde{\psi}_{ND}(\cdot,x,\cdot)\right),\end{aligned} \tag{46}$$

where θ stands for the usual Heaviside function, and ψ^-, ψ_{DN}, ψ_{ND}, $\tilde{\psi}_{DN}$ and $\tilde{\psi}_{ND}$ are respectively defined by (33), (35), (36), (42) and (41).

Let us now establish that the transversal modes associated with $n \geq n_1 + 1$, appearing in the decomposition of $\psi(t,\cdot,\cdot)$, vanish as $t \to \pm\infty$. In view of (32), (35)-(36) and (46), it is enough to examine the functions $\tilde{\psi}_{DN}$ and $\tilde{\psi}_{ND}$. Applying Fubini Theorem, we obtain that

$$\|\tilde{\psi}_{ND}(t,\cdot,\cdot)\|^2_{L^2(\Omega)} = \int_{\mathbb{R}_+} \sum_{n=n_1+1}^{\infty} \left| \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} t_n(k) e^{-\kappa_n(k)x} dk \right|^2 dx, \tag{47}$$

since $\{\chi_n^{(+)},\ n \geq 1\}$ is an orthornomal basis of $L^2(0,d)$. Further we get

$$\begin{aligned}&\int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} t_n(k) e^{-\kappa_n(k)x} dk\\ &= \frac{1}{2it} \int_{\mathbb{R}} e^{-i(\mu_{n_0}+k^2)t} \frac{\partial}{\partial k}\left(k^{-1} a(k) t_n(k) e^{-\kappa_n(k)x}\right) dk,\ x \in \mathbb{R}_+,\ t > 0,\end{aligned}$$

by integrating by parts. Taking into account that $a \in C^1(\mathbb{R})$ is supported in $[\alpha,\beta]$, with $\alpha > 0$, that $t_n(k)$ satisfies the estimate (40), that

$$\frac{dt_n}{dk}(k) = \frac{d}{dk}(\chi_n^+, \varphi(k))_{L^2(0,d)} = \left(\chi_n^+, \frac{\partial\varphi}{\partial k}(k)\right)_{L^2(0,d)},$$

where $k \mapsto \frac{\partial\varphi}{\partial k}(k) \in C^0(\mathbb{R}_+^*, \mathcal{H}^{\frac{1}{2}})$ from Theorem 2, and that $\kappa_n(k) \geq \kappa_n(\beta)$ for all $k \in [\alpha,\beta]$, we find out two positive constants d_1 and d_2, both of them being independent of n, such that the estimate

$$\left| \int_{\mathbb{R}} a(k) e^{-i(\mu_{n_0}+k^2)t} t_n(k) e^{-\kappa_n(k)x} dk \right| \leq \frac{d_1 + d_2 x}{2|t|\sqrt{n}} e^{-\kappa_n(\beta)x},$$

holds uniformly in $t \in \mathbb{R}^*$ and $x \in \mathbb{R}_+^*$. From this and (47) then follows that

$$\|\tilde{\psi}_{ND}(t,\cdot,\cdot)\|^2_{L^2(\Omega)} \leq \frac{c}{|t|},\ t \in \mathbb{R}^*, \tag{48}$$

for some constant $c > 0$, which does not depend on t. Arguing in the same way we get in addition that

$$\|\tilde{\psi}_{DN}(t,\cdot,\cdot)\|^2_{L^2(\Omega)} \leq \frac{c}{|t|},\ t \in \mathbb{R}^*. \tag{49}$$

The next step of the proof involves estimating $\|\psi^-(t,\cdot,\cdot) - \psi_{ND}(t,\cdot,\cdot)\|_{L^2(\mathbb{R}^*_+\times(0,d))}$ for $t < 0$. Recalling (33) and (36), we get

$$\begin{aligned}
&\psi^-(t,x,y) - \psi_{ND}(t,x,y)\\
&= \int_{\mathbb{R}} a(k)e^{-i(\mu_{n_0}+k^2)t}\sum_{l=1}^{n_1} e^{ik_l x}\left(\delta_{ln_0}\chi_l^-(y) - t_l(k)\chi_l^+(y)\right)dk\\
&= -\sum_{l=1}^{n_1}\int_{\mathbb{R}} e^{i\left(k_l x-(\mu_{n_0}+k^2)t\right)}\frac{\partial q_l}{\partial k}(k,t,x,y)dk,
\end{aligned}$$

upon integrating by parts, where

$$q_l(k,t,x,y) = \frac{a(k)}{i(-2kt + kk_l^{-1}x)}(\delta_{ln_0}\chi_l^-(y) - t_l(k)\chi_l^+(y)).$$

From this and (4) then follows that

$$|\psi^-(t,x,y) - \psi_{ND}(t,x,y)| \leq \frac{e_1}{x - 2k_{n_1}(\alpha)t} + \frac{e_2x - e_3t}{(x - 2k_{n_1}(\alpha)t)^2},$$

for $t < 0$, $x > 0$ and $y \in (0,d)$, where e_1, e_2 and e_3 are three positive constants which are independent of t, x and y. As a consequence we may find $c > 0$, such that for all $t < 0$, we have

$$\|\psi^-(t,\cdot,\cdot) - \psi_{ND}(t,\cdot,\cdot)\|^2_{L^2(\mathbb{R}^*_+\times(0,d))} \leq \frac{c}{|t|}. \tag{50}$$

Analogously, recalling from Theorem 2 that $k \mapsto r_l(k)$ and $k \mapsto t_l(k)$ are smooth for all $l = 0,\ldots,n_1$, we get for every $t < 0$ that

$$\|\psi_{DN}(t,\cdot,\cdot)\|^2_{L^2(\mathbb{R}^*_-\times(0,d))} \leq \frac{c}{|t|}. \tag{51}$$

Now, since

$$\begin{aligned}
&\|\psi(t,\cdot,\cdot) - \psi^-(t,\cdot,\cdot)\|^2_{L^2(\Omega)}\\
&\leq \|\psi^-(t,\cdot,\cdot) - \psi_{ND}(t,\cdot,\cdot)\|^2_{L^2(\mathbb{R}^*_+\times(0,d))} + \|\psi_{DN}(t,\cdot,\cdot)\|^2_{L^2(\mathbb{R}^*_-\times(0,d))}\\
&+ \|\tilde{\psi}_{DN}(t,\cdot,\cdot)\|^2_{L^2(\Omega)} + \|\tilde{\psi}_{ND}(t,\cdot,\cdot)\|^2_{L^2(\Omega)},
\end{aligned}$$

from (46), we obtain the desired result for $t \to -\infty$ by putting (48)–(51) together.

Similarly, arguing as above for $t > 0$, by means of the decomposition

$$\psi(\cdot, x, \cdot) = \psi^+(\cdot, x, \cdot) + \theta(x)\tilde{\psi}_{ND}(\cdot, x, \cdot) + \theta(-x)\left(\psi^-(\cdot, x, \cdot) + \tilde{\psi}_{DN}(\cdot, x, \cdot)\right),$$

we obtain the desired result for $t \to +\infty$.

□

As seen in the proof of (45), $\|\psi(t, \cdot, \cdot) - \psi^{\pm}(t, \cdot, \cdot)\|_{L^2(\Omega)}$ scales like $\mathcal{O}(t^{-1/2})$. Actually, this is due to the fact that a is C^1, as a smoother a would allow for several integrations by parts, and consequently for a faster time decay.

Further, assumption (30) guarantees that the quasi-momenta involved in the framework of in Theorem 3 remain separated from the discrete threshold momentum values of M. This is not a very strong restriction when studying the scattering of particles with momentum close to given value of $k > 0$, which is sufficient for the definition of reflection and transmission coefficients, as the skipped threshold points form a zero measure set where the reflection and transmission coefficients need not necessarily be defined. However, their behavior near the thresholds, which we do not attempt to study in this paper, is certainly a point of interest.

IV. NUMERICAL RESULTS

For the illustration, we present here also numerically computed transition probabilities. Recall that reflection and transmission probability densities from the initial state of transversal mode n_0 and longitudinal momentum k to the final transversal mode m are

$$PRm = \frac{k_m(k)}{k}|r_m(k)|^2 \quad , \quad PTm = \frac{k_m(k)}{k}|t_m(k)|^2 \quad .$$

The matching conditions were cut to the finite number of transversal modes, projected on a suitable finite-dimensional basis, and the resulting system of linear equations for the reflection and transmission coefficients solved numerically. No attempt to prove the convergence of this procedure was done, the precision was tested only numerically.

The computed probability densities for $n_0 = 1, 2$ are shown in Figures 2 and 3. They seem to be continuous but not smooth at the thresholds where excitations of the further transversal modes in the final state are opened. The total reflection at $k \to 0$ is seen in accordance with the Dirichlet decoupling at $d \to 0$ proved by Borisov and Cardone[10] (notice, that the dimesionless value of kd is a relevant parameter).

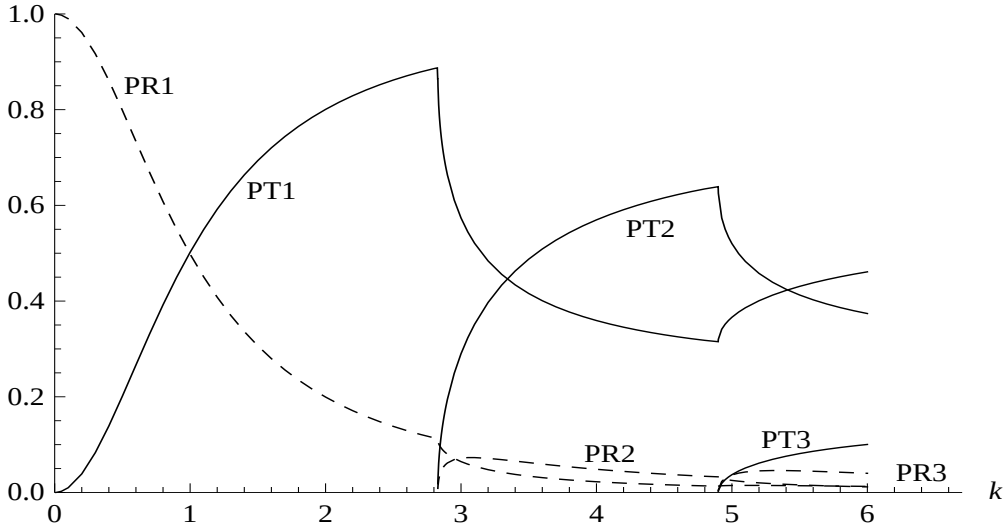

FIG. 2. Reflection (dashed) and transmission probabilities PRm and PTn from the initial transversal state $n_0 = 1$ and longitudinal momentum k (in units of $\frac{\pi}{2d}$) to the transversal states m and n respectively.

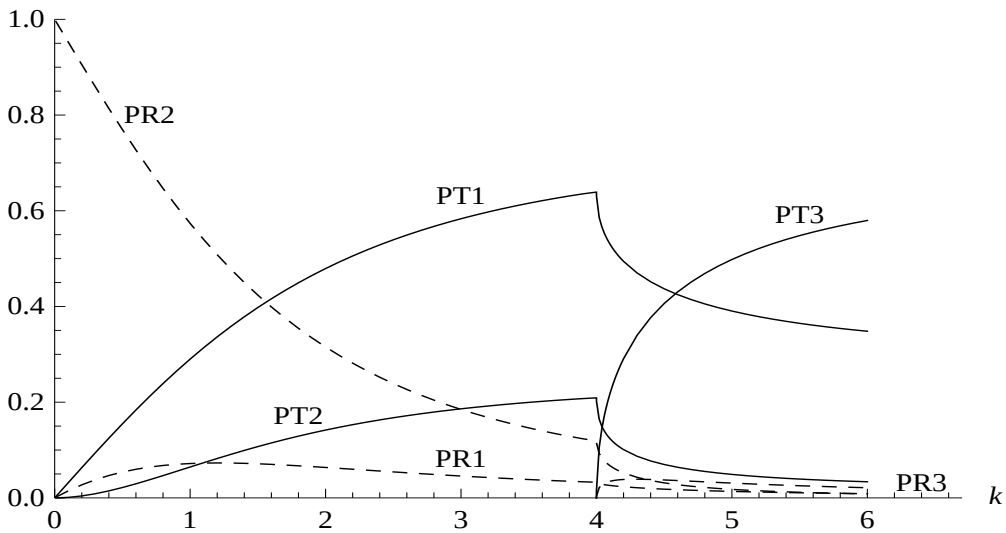

FIG. 3. Reflection (dashed) and transmission probabilities PRm and PTn from the initial transversal state $n_0 = 2$ and longitudinal momentum k (in units of $\frac{\pi}{2d}$) to the transversal states m and n respectively.

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Appendix A: Proof of lemma 1

The proof is by means of the two following technical lemmas. With the notation (20), we shall also write $P_N^{\pm} = \sum_{n=1}^N p_n^{\pm}$.

1. Preliminary results

Lemma 2 *Let $N \in \mathbb{N}^*$. Then there exists $\epsilon_N \in (0,1)$ such that we have*

$$\min\left(\|P_N^+\varphi\|_{L^2(0,d)}, \|P_N^-\varphi\|_{L^2(0,d)}\right) \leq \varepsilon_N \|\varphi\|_{L^2(0,d)}, \ \varphi \in \mathcal{P}_N.$$

Proof. Let us first establish that $\{\chi_n^{\pm},\ n = 1, \ldots, N\}$ is linearly independent. We consider $2N$ complex numbers $\alpha_n^{\pm}$ for $n = 1, \ldots, N$ such that $\sum_{n=1}^N (\alpha_n^+\chi_n^+ + \alpha_n^-\chi_n^-) = 0$. Differentiating $2r$-times, $r \in \mathbb{N}$, we get that

$$\sum_{n=1}^N \mu_n^r(\alpha_n^+\chi_n^+ + \alpha_n^-\chi_n^-) = 0.$$

Evaluating this identity at $x = 0$, we obtain $\sum_{n=1}^N \mu_n^r\alpha_n^+ = 0$. The determinant of the system formed by the above equations with $r = 0, \ldots, N-1$, is Vandermonde and equals $\prod_{1\leq r<s\leq N}(\mu_s - \mu_r) > 0$. Therefore $\alpha_n^+ = 0$ for all $n = 1, \ldots, N$. Arguing as before with $x = d$ we obtain that $\alpha_n^- = 0$ for $n = 1, \ldots, N$, showing that the vectors $\chi_n^{\pm}$, for $n = 1, \ldots, N$, are linearly independent.

Assuming that the statement of the Lemma does not hold, there would be a sequence $\{\varphi_n,\ n \in \mathbb{N}^*\} \in (\mathcal{P}_N)^{\mathbb{N}^*}$ such that

$$\|\varphi_n\|_{L^2(0,d)} = 1 \text{ and } \min(\|P_N^+\varphi_n\|_{L^2(0,d)}, \|P_N^-\varphi_n\|_{L^2(0,d)}) > 1 - \frac{1}{n},$$

for every $n \in \mathbb{N}^*$. As the unit sphere in the finite dimensional linear space $\mathcal{P}_N$ is compact, we may find a subsequence that converges to a limit $\varphi_0 \in \mathcal{P}_N$ obeying

$$\|\varphi_0\|_{L^2(0,d)} = \|P_N^+\varphi_0\|_{L^2(0,d)} = \|P_N^-\varphi_0\|_{L^2(0,d)} = 1.$$

Thus we have $P_N^+\varphi_0 = \varphi_0 = P_N^-\varphi_0$. Since $\{\chi_n^\pm,\ n = 1, \dots, N\}$ is linearly independent, then $\varphi_0 = 0$, contradicting the fact that $\|\varphi_0\|_{L^2(0,d)} = 1$. As a consequence the statement is true for every $\varphi \in \mathcal{P}_N$ such that $\|\varphi\|_{L^2(0,d)} = 1$. Therefore it holds for any $\phi \in \mathcal{P}_N$ since it is valid for $\phi = 0$ and for $\phi/\|\phi\|_{L^2(0,d)}$ when $\phi \neq 0$.

□

Lemma 3 *Let $N \in \mathbb{N}^*$. Then there exists $\eta_N \in (0,1)$ such that the estimate*

$$\max\left(\|(I - P_N^+)\phi\|_{L^2(0,d)}, \|(I - P_N^-)\phi\|_{L^2(0,d)}\right) \geq \eta_N \|\phi\|_{L^2(0,d)},$$

holds for all $\phi \in L^2(0,d)$.

Proof. The proof boils down to the fact that

$$\begin{aligned}\|(I - P_N^\pm)\phi\|^2_{L^2(0,d)} &= \|\phi\|^2_{L^2(0,d)} - \|P_N^\pm\phi\|^2_{L^2(0,d)} \\ &= \|\phi\|^2_{L^2(0,d)} - \|P_N^\pm P_N\phi\|^2_{L^2(0,d)},\end{aligned}$$

and $\|\phi\|^2_{L^2(0,d)} = \|(I - P_N)\phi\|^2_{L^2(0,d)} + \|P_N\phi\|^2_{L^2(0,d)}$. Indeed, this entails

$$\begin{aligned}&\max\left(\|(I - P_N^+)\phi\|^2_{L^2(0,d)}, \|(I - P_N^-)\phi\|^2_{L^2(0,d)}\right) \\ &= \|(I - P_N)\phi\|^2_{L^2(0,d)} + \|P_N\phi\|^2_{L^2(0,d)} \\ &\quad - \min\left(\|P_N^+P_N\phi\|^2_{L^2(0,d)}, \|P_N^-P_N\phi\|^2_{L^2(0,d)}\right),\end{aligned}$$

which, together with Lemma 2, yields

$$\begin{aligned}&\max\left(\|(I - P_N^+)\phi\|^2_{L^2(0,d)}, \|(I - P_N^-)\phi\|^2_{L^2(0,d)}\right) \\ &\geq \|(I - P_N)\phi\|^2_{L^2(0,d)} + (1 - \epsilon_N^2)\|P_N\phi\|^2_{L^2(0,d)}.\end{aligned}$$

Since the right hand side of the above estimate is lower bounded by $(1 - \epsilon_N^2)\|\phi\|^2_{L^2(0,d)}$, we obtain the desired result.

□

2. Completion of the proof

For all $\phi \in \mathcal{H}^{\frac{1}{2}}$, we have

$$(D_2\phi, \phi)_{-\frac{1}{2},\frac{1}{2}} = \sum_{n=n_1+1}^{\infty} \kappa_n \left((p_n^-\phi, \phi)_{L^2(0,d)} + (p_n^+\phi, \phi)_{L^2(0,d)}\right),$$

from (22), so we get

$$\begin{aligned}(D_2\phi,\phi)_{-\frac{1}{2},\frac{1}{2}} &\geq \kappa_{n_1+1}\left(\|(I-P_{n_1}^-)\phi\|^2_{L^2(0,d)}+\|(I-P_{n_1}^+)\phi\|^2_{L^2(0,d)}\right)\\ &\geq \kappa_{n_1+1}\eta^2_{n_1}\|\phi\|^2_{L^2(0,d)},\end{aligned} \tag{A1}$$

by Lemma 3, showing that D_2 is injective.

To prove that D_2 is a surjection, we first establish the two following lemmas.

Lemma 4 *For each $\psi\in\mathcal{H}^{-\frac{1}{2}}$, the functional*

$$F_\psi(\phi)=(D_2\phi,\phi)_{-\frac{1}{2},\frac{1}{2}}-2\Re(\psi,\phi)_{-\frac{1}{2},\frac{1}{2}}$$

is real-valued, strictly convex, continuous and coercive on $\mathcal{H}^{\frac{1}{2}}$.

Proof. First, it is apparent from the definition of F_ψ that $F_\psi(\phi)\in\mathbb{R}$ for all $\phi\in\mathcal{H}^{\frac{1}{2}}$.

Next, we get through direct calculation that

$$\begin{aligned}&tF_\psi(\phi_1)+(1-t)F_\psi(\phi_2)-F_\psi(t\phi_1+(1-t)\phi_2)\\ &=t(1-t)(D_2(\phi_1-\phi_2),\phi_1-\phi_2)_{-\frac{1}{2},\frac{1}{2}},\end{aligned}$$

for each $t\in[0,1]$ and all $\phi_1,\phi_2\in\mathcal{H}^{\frac{1}{2}}$. This and (A1) yield that F_ψ is strictly convex.

Further, $\|D_2\delta\|_{-\frac{1}{2}}$ being majorized, up to some multiplicative positive constant, by $\|\delta\|_{\frac{1}{2}}$, uniformly in $\delta=\sum_{n=1}^{+\infty}\delta_n^\pm\chi_n^\pm\in\mathcal{H}^{\frac{1}{2}}$, as can be seen from the following computation arising from (5),

$$\begin{aligned}\|D_2\delta\|^2_{-\frac{1}{2}} &= \sum_{n=n_1+1}^{+\infty}\frac{\kappa_n^2}{n}\left(|\delta_n^+|^2+|\delta_n^-|^2\right)\\ &\leq \frac{\pi^2}{d^2}\sum_{n=n_1+1}^{+\infty}\frac{n^2-n_0^2}{n}\left(|\delta_n^+|^2+|\delta_n^-|^2\right)\\ &\leq \frac{\pi^2}{d^2}\sum_{n=n_1+1}^{+\infty}n\left(|\delta_n^+|^2+|\delta_n^-|^2\right)\leq\frac{\pi^2}{d^2}\|\delta\|^2_{\frac{1}{2}},\end{aligned}$$

the continuity of F_ψ follows readily from the basic estimate

$$\begin{aligned}&|F_\psi(\phi+\delta)-F_\psi(\phi)|\\ &\leq 2\left|\Re(D_2\phi,\delta)_{-\frac{1}{2},\frac{1}{2}}-\Re(\psi,\delta)_{-\frac{1}{2},\frac{1}{2}}\right|+(D_2\delta,\delta)_{-\frac{1}{2},\frac{1}{2}}\\ &\leq 2\left(\|D_2\phi\|_{-\frac{1}{2}}+\|\psi\|_{-\frac{1}{2}}+\|D_2\delta\|_{-\frac{1}{2}}\right)\|\delta\|_{\frac{1}{2}},\end{aligned}$$

which holds true for any $\phi\in\mathcal{H}^{\frac{1}{2}}$.

Let us now prove that F_ψ is coercive. We use (5), getting $\kappa_n \geq \frac{\kappa_{n_1+1}}{n_1+1} n$ for every $n \geq n_1+1$, hence

$$(D_2\phi, \phi)_{-\frac{1}{2},\frac{1}{2}} \geq \frac{\kappa_{n_1+1}}{n_1+1} \sum_{n=n_1+1}^{\infty} n(|a_n^+|^2 + |a_n^-|^2), \tag{A2}$$

for all $\phi = \sum_{n=1}^{\infty} a_n^\pm \chi_n^\pm \in \mathcal{H}^{\frac{1}{2}}$. Further, since

$$\sum_{n=n_1+1}^{+\infty} n(|a_n^+|^2 + |a_n^-|^2) \geq (n_1+1) \sum_{n=n_1+1}^{+\infty} (|a_n^+|^2 + |a_n^-|^2),$$

we derive from Lemma 3 that

$$\begin{aligned}\sum_{n=n_1+1}^{+\infty} n(|a_n^+|^2 + |a_n^-|^2) &\geq \frac{n_1+1}{2} \eta_{n_1}^2 \sum_{n=1}^{+\infty} (|a_n^+|^2 + |a_n^-|^2) \\ &\geq \frac{n_1+1}{2n_1} \eta_{n_1}^2 \sum_{n=1}^{n_1} n(|a_n^+|^2 + |a_n^-|^2).\end{aligned}$$

Bearing in mind that $\eta_{n_1} \in (0,1)$, this entails that

$$\sum_{n=n_1+1}^{+\infty} n(|a_n^+|^2 + |a_n^-|^2) \geq \frac{n_1+1}{3n_1+1} \eta_{n_1}^2 \|\phi\|_{\frac{1}{2}}^2,$$

for all $\phi \in \mathcal{H}^{\frac{1}{2}}$. From this and (A2) then follows that

$$(D_2\phi, \phi)_{-\frac{1}{2},\frac{1}{2}} \geq \frac{\kappa_{n_1+1}}{3n_1+1} \eta_{n_1}^2 \|\phi\|_{\frac{1}{2}}^2, \ \phi \in \mathcal{H}^{\frac{1}{2}},$$

showing that F_ψ is coercive.

□

Lemma 5 *Let ψ and F_ψ be the same as in Lemma 4. Assume that F_ψ has its minimum at $\phi \in \mathcal{H}^{\frac{1}{2}}$. Then we have*

$$D_2\phi = \psi \ in \ \mathcal{H}^{-\frac{1}{2}}. \tag{A3}$$

Proof. Fix $\delta \in \mathcal{H}^{\frac{1}{2}}$. The function $\mathbb{R} \ni t \mapsto F_\psi(\phi + t\delta)$ has a minimum at $t = 0$, by assumption, so its derivative is zero there. As

$$F_\psi(\phi + t\delta) = F_\psi(\phi) + 2t\Re(D_2\phi - \psi, \delta)_{-\frac{1}{2},\frac{1}{2}} + t^2(D_2\delta, \delta)_{-\frac{1}{2},\frac{1}{2}},$$

this means that $\Re(D_2\phi - \psi, \delta)_{-\frac{1}{2},\frac{1}{2}} = 0$. Further, substituting $i\delta$ for δ in this equation, we find out that

$$(D_2\phi - \psi, \delta)_{-\frac{1}{2},\frac{1}{2}} = 0,$$

which entails (A3) since δ is arbitrary in $\mathcal{H}^{\frac{1}{2}}$.

$\square$

We are now in position to prove the first assertion in Lemma 1. For ψ in $\mathcal{H}^{-\frac{1}{2}}$ fixed, we know from Lemma 4 that F_ψ admits a unique minimum $\phi \in \mathcal{H}^{\frac{1}{2}}$ (see e.g.[13]), which is solution to (A3), according to Lemma 5. This establishes that D_2 is surjective, and thus one-to-one from $\mathcal{H}^{\frac{1}{2}}$ onto $\mathcal{H}^{-\frac{1}{2}}$, since it is already known to be injective. Moreover, the boundedness of D_2^{-1} follows from the inverse mapping theorem (e.g.[12][Theorem III.11]).

Last, we prove that the operator $(D_2^{-1})_{|L^2(0,d)}$ is symmetric. We pick $f, g \in \mathcal{H}^{-\frac{1}{2}}$ and recall from (22) that $(D_2 u, v)_{-\frac{1}{2},\frac{1}{2}} = \overline{(D_2 v, u)}_{-\frac{1}{2},\frac{1}{2}}$ for every $u, v \in \mathcal{H}^{\frac{1}{2}}$. Taking $u = D_2^{-1} f$ and $v = D_2^{-1} g$ in this equation we get that

$$(f, D_2^{-1} g)_{-\frac{1}{2},\frac{1}{2}} = \overline{(g, D_2^{-1} f)}_{-\frac{1}{2},\frac{1}{2}}. \tag{A4}$$

In the peculiar case where $f, g \in L^2(0,d)$, we have $(f, D_2^{-1} g)_{-\frac{1}{2},\frac{1}{2}} = (f, D_2^{-1} g)_{L^2(0,d)}$ and $(g, D_2^{-1} f)_{-\frac{1}{2},\frac{1}{2}} = (g, D_2^{-1} f)_{L^2(0,d)}$, hence

$$(f, D_2^{-1} g)_{L^2(0,d)} = (D_2^{-1} f, g)_{L^2(0,d)},$$

from (A4), which is the required symmetry relation.

Appendix B: Limits in matching conditions

This appendix is devoted to proving that the limit (13) coincides with the right hand side of (14). To do that we start by establishing that

(i) $\frac{\partial \varphi}{\partial x}(\pm\varepsilon, \cdot)$ goes to $\frac{\partial \varphi}{\partial x}(0, \cdot)$ in $L^2(0,d)$ as $\varepsilon \downarrow 0$;

(ii) $f(k, \pm\varepsilon, \cdot)$ tends to $f(k, 0^\pm, \cdot)$ in $L^2(0,d)$ as $\varepsilon \downarrow 0$.

First, we notice for every $y \in (0,d)$ and $\varepsilon > 0$ that

$$\left| \frac{\partial \varphi}{\partial x}(\pm\varepsilon, y) - \frac{\partial \varphi}{\partial x}(0, y) \right| \leq \left\| \frac{\partial^2 \varphi}{\partial x^2} \right\|_{L^\infty(\Omega)} \varepsilon,$$

so we get

$$\left\| \frac{\partial \varphi}{\partial x}(\pm\varepsilon, \cdot) - \frac{\partial \varphi}{\partial x}(0, \cdot) \right\|_{L^2(0,d)} \leq \left\| \frac{\partial^2 \varphi}{\partial x^2} \right\|_{L^\infty(\Omega)} \sqrt{d}\varepsilon,$$

which entails (i).

For the second statement (ii), we shall only prove that $\lim_{\varepsilon\downarrow 0} f(k,-\varepsilon,\cdot) = f(k,0^-,\cdot)$ in $L^2(0,d)$, the case of the limit from the right being fully analogical. From the definition of the trace $f(k,0^-,\cdot)$, we may find $L>0$, $\varepsilon_0>0$ and a sequence of functions $(f_n)_{n\geq 1}$ in $C^\infty(\Omega)$ satisfying

$$\lim_{n\to+\infty} \|f_n - f(k,\cdot,\cdot)\|_{H^1((-L-\varepsilon_0,0)\times(0,d))} = 0, \tag{B1}$$

such that $f_n(0,\cdot)$ tends to $f(k,0^-,\cdot)$ in $\mathcal{H}^{\frac{1}{2}}$ as n goes to infinity. Moreover we have

$$\|f_n(0,\cdot) - f(k,0^-,\cdot)\|_{\frac{1}{2}} \leq c\|f_n - f(k,\cdot,\cdot)\|_{H^1((-L,0)\times(0,d))},$$

for some positive constant c which is independent of f and f_n. Further, since $\|f(k,-\varepsilon,\cdot) - f(k,0^-,\cdot)\|_{\frac{1}{2}}$ is majorized by the sum

$$\|f(k,-\varepsilon,\cdot) - f_n(-\varepsilon,\cdot)\|_{\frac{1}{2}} + \|f_n(-\varepsilon,\cdot) - f_n(0,\cdot)\|_{\frac{1}{2}} + \|f_n(0,\cdot) - f(k,0^-,\cdot)\|_{\frac{1}{2}},$$

for every $\varepsilon\in(0,\varepsilon_0)$, we get that

$$\begin{aligned} &c^{-1}\|f(k,-\varepsilon,\cdot) - f(k,0^-,\cdot)\|_{\frac{1}{2}} \\ &\leq \|f(k,\cdot,\cdot) - f_n\|_{H^1((-L-\varepsilon,-\varepsilon)\times(0,d))} + \|f_n(\cdot-\varepsilon,\cdot) - f_n(\cdot,\cdot)\|_{H^1((-L,0)\times(0,d))} \\ &+ \|f_n - f(k,\cdot,\cdot)\|_{H^1((-L,0)\times(0,d))}. \end{aligned} \tag{B2}$$

In light of (B1), the first and third terms in the right hand side of (B2) can de made arbitrarily small upon chosing n sufficiently large. For such an n, using the uniform continuity of the function f_n or applying[14] [Chapter 1, Lemma 3.5], it is possible to make the second term arbitrarily small by taking $\varepsilon>0$ small enough. As a consequence we have $\lim_{\varepsilon\downarrow 0} f(k,-\varepsilon,\cdot) = f(k,0^-,\cdot)$ in $\mathcal{H}^{\frac{1}{2}}$, and thus in $L^2(0,d)$, which is the statement of (ii).

Putting (i) and (ii) together, we obtain that

$$\begin{aligned} &\lim_{\varepsilon\downarrow 0}\left(\int_0^d \bar{f}(k,-\varepsilon,y)\frac{\partial\varphi}{\partial x}(-\varepsilon,y)dy - \int_0^d \bar{f}(k,\varepsilon,y)\frac{\partial\varphi}{\partial x}(\varepsilon,y)dy\right) \\ &= \left(f(k,0^-,\cdot) - f(k,0^+,\cdot), \frac{\partial\varphi}{\partial x}(0,\cdot)\right)_{L^2(0,d)}. \end{aligned} \tag{B3}$$

The rest of the proof is to compute $\int_0^d \frac{\partial\bar{f}}{\partial x}(k,\pm\varepsilon,\cdot)\varphi(\pm\varepsilon,y)dy$ as $\varepsilon\downarrow 0$. We shall actually restrict ourselves to calculating the limit from the left, the other case being fully analogical. To do that we start by decomposing $\varphi(-\varepsilon,\cdot)\in\mathcal{H}_-^{\frac{1}{2}}$, as

$$\varphi(-\varepsilon,\cdot) = \sum_{n=1}^{\infty} b_n(-\varepsilon)\chi_n^-,\ b_n(-\varepsilon) = \int_0^d \chi_n^-(y)\varphi(-\varepsilon,y)dy,\ n\in\mathbb{N}^*,$$

and notice from (1) upon integrating several times by parts, that

$$|b_n(-\varepsilon)| = \left| \int_0^d \chi_n^-(y)\varphi(-\varepsilon, y)\, dy \right| \leq \frac{c}{\mu_n^2}, \ c = \sqrt{2d} \left\| \frac{\partial^4 \varphi}{\partial y^4} \right\|_{L^\infty(\Omega)}.$$

Further, it follows from (7) and (15) that

$$\begin{aligned} &\int_0^d \frac{\partial \bar{f}}{\partial x}(k, -\varepsilon, y)\varphi(-\varepsilon, y)dy - (f_x(k, 0^-, \cdot), \varphi(0, \cdot))_{-\frac{1}{2}, \frac{1}{2}} \\ &= -ik(b_{n_0}(0) - b_{n_0}(-\varepsilon)e^{-ik\varepsilon}) + i\sum_{l=1}^{n_1} k_l \overline{r_l}(b_l(0) - b_l(-\varepsilon))e^{ik_l\varepsilon}) \\ &- \sum_{n=n_1+1}^{\infty} \kappa_n \overline{r_n}(b_n(0) - b_n(-\varepsilon)e^{-k_n\varepsilon}), \end{aligned} \tag{B4}$$

from where we get

$$\begin{aligned} &\left| \int_0^d \frac{\partial \bar{f}}{\partial x}(k, -\varepsilon, y)\varphi(-\varepsilon, y)dy - (f_x(k, 0^-, \cdot), \varphi(0, \cdot))_{-\frac{1}{2}, \frac{1}{2}} \right| \\ &\leq \frac{2ck}{\mu_{n_0}^2} + 2c\sum_{l=1}^{n_1} \frac{k_l|r_l|}{\mu_l^2} + 2c\sum_{n=n_1+1}^{\infty} \frac{\kappa_n|r_n|}{\mu_n^2}. \end{aligned}$$

Bearing in mind that μ_n scales like n^2, and recalling (5) and (10), we see that the series in the above expression is convergent. Thus we obtain

$$\lim_{\varepsilon \downarrow 0} \int_0^d \frac{\partial \bar{f}}{\partial x}(k, -\varepsilon, y)\varphi(-\varepsilon, y)dy = (f_x(k, 0^-, \cdot), \varphi(0, \cdot))_{-\frac{1}{2}, \frac{1}{2}},$$

by taking the limit $\varepsilon \to 0^+$ term by term in (B4) and using the continuity of $\varepsilon \mapsto b_n(-\varepsilon)$ at 0. Now the desired result follows from this and (B3).

REFERENCES

[1]D. V. Evans, M. Levitin, D. Vassiliev, *J. Fluid Mech.* **261**, 21 (1994).

[2]P. Exner, P. Šeba, M. Tater, D. Vaněk, *J. Math. Phys.* **37**, 4867 (1996).

[3]P. Exner, S. A. Vugalter, *Ann. Inst. H. Poincaré - Phys. Theor.* **65**, 109 (1996).

[4]J. Dittrich, J. Kříž, *J. Math. Phys.* **43**, 3892 (2002).

[5]H. Kovařík, D. Krejčiřík, *Math. Nachr.* **281**, 1159 (2008).

[6]D. Borisov, G. Cardone, *J. Math. Phys.* **52**, 123513 (2011).

[7]H. Najar, O. Olendski, *J. Phys. A* **44**, 305304 (2011).

[8]D. Krejčiřík, E. Zuazua, *J. Diff. Eq.* **250**, 2334 (2011).

[9]D. Borisov, R. Bunoiu, G. Cardone, *Ann. H. Poincaré* **11**, 1591 (2010); *C. R. Acad. Sci. Paris, Ser. I* **349**, 53 (2011).

[10]D. Borisov, G. Cardone, *J. Math. Phys.* **53**, 023503 (2012).

[11]M. S. Birman, G. E. Skvortsov, *IVUZ, Mat.* **30**(5), 12 (1962).

[12]M. Reed, B. Simon, *Methods of Modern Mathematical Physics. I. Functional Analysis* (Academic Press, New York, 1980).

[13]A. Jaffe, C. Taubes, *Vortices and Monpoles* (Birkhäuser, Boston, 1980).

[14]C. Zuily, *Éléments de distributions et d'équations aux dérivées partielles* (Dunod, Paris, 2002).