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CONFINEMENT EFFECTS ON SCATTERING FOR A NANOPARTICLE

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The motion of a nanoparticle in a narrow, bend channel is used to illustrate features of scattering in systems with semi-open geometries. Under certain general constraints on the geometry, results on the scattering process are established.

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1. Introduction

Propagation of waves in bent structures is a classic topic in the theory of guided waves [1]. A new and very exciting source of problems has recently appeared in quantum mechanics, arising from todays possibility to produce electrically conducting structures of ever smaller size by nanofabrication techniques. The concept of wave propagation through crosses and bent wires is also relevant for such mesoscopic systems [2, 3], which are expected to become the building blocks of the next-generation electronics [4, 5].

A pressing challenge in this emerging area of applied physics is to investigate properties (bound states, quasi-bound states, and scattering processes) of these quantum systems, in particular the Quantum Wire (QW) which is a narrow two-dimensional conducting surface which permits electrons to propagate in the channels formed by this surface, but reguire the electron wave function to vanish on the boundary of the surface (Dirichlet boundary conditions). Since the width of the QW is roughly equal to the de Broglie wavelength of a cold electron, wave effects will dominate the physics of the system. As a consequence, quantum interference effects have been studied extensively by means of QWs and in recent years hundreds of papers have discussed the basic and applied physics of such quantum heterostructures [6–9]. The most simple system is a strip Σ of infinite extent with a bend in the center and open straight ends. The corresponding Hamiltonian, denoted by L, of the system is chosen as a multiple of the Dirichlet Laplacian on the strip; this corresponds to infinitely hard walls at the boundary $\partial\Sigma$. No "classically forbidden" region exists for such a system and it thus came as a surprise that they possess a bound state [10]. Remarkably, it was later shown [11] that at least one bound state exists for *any* two-dimensional surface of constant width; excluding surfaces of constant curvature, which have no bound states. A qualitative explanation can be found in [8]. Many efforts have thus been devoted to bound states in bent QWs (see [8] and references therein), even taking into account external fields [12–14].

A key problem of solid-state electronics is understanding various collision processes present in semiconductors and semiconductor structures. Many processes exist, *e.g.*, electron interactions with bulklike and confined phonons, crystals defects and imperfections, and neutral and ionized impurities [6–9]. In quantum structures these collision mechanisms can be significantly different from those in bulk materials. We shall focus on one such mechanism, generated by bending and occuring for a fairly large class of QWs.

Perhaps surprisingly, for systems which have been so widely studied, very few papers exist on scattering theory. Quantum scattering theory is the subfield of quantum mechanics which concerns the large-time asymptotics of the solutions of the Schrödinger equation and with the structure of the continuous spectrum of the corresponding Schrödinger operator. One of its main problems is to prove (or disprove) *asymptotic completeness*, which roughly speaking, is a statement that all solutions of the Schrödinger equation under consideration must follow asymptotically certain prescribed patterns. Proving asymptotic completeness is the first step in a detailed investigation of scattering properties of any quantum system. Typically, applied physicists enter after this step and the literature on computation of scattering properties in QWs is indeed vast. For arbitrary shaped wires, such computations require numerical solution of the two-dimensional Helmholz equation to allow one to extract the transmission amplitudes. Numerous techniques have been invented to solve this equation, *e.g.* wave function matching methods [10, 15] (for simple geometries), Green function techniques [6, 7, 16, 17], and mode matching [18–20].

Our objective is to go one step further in the foundations underpinning the physics of scattering for a wide class of QWs. The description of the quantum theory of scattering (see, *e.g.* [21]) closely parallels the classical formalism. In lieu of the classical orbit obeying Newton's equation, we have a state vector $\psi(t)$ satisfying the time-dependent Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H\psi(t)\,, \qquad \psi(0) = \psi_0\,. \tag{1.1}$$

The solution to (1.1) is given by $\psi(t) = U(t)\psi_0 = e^{-itH}\psi_0$, where $U(t)$ is the so-called evolution operator (defined via the spectral theorem), and ψ_0 is any vector in the appropiate Hilbert space $\mathcal{H}$. In quantum scattering theory one often has a "free" Hamiltonian H_0 and a potential V such that the "perturbed" Hamiltonian is $H = H_0 + V$. For suitable initial data ψ_0, the solution $U(t)\psi_0$ propagates from the region where the perturbation V is large and we expect that it should be approximated well as $t \to \pm\infty$ by the solutions $e^{-itH_0}\phi_\pm$ of the unperturbed Schrödinger equation; the free evolution e^{-itH_0} is denoted $U_0(t)$. The solution $\psi(t)$ describes a process in which the system, described by the asymptotic state ϕ_- in the distant past, interacts with the perturbation and is changed into the asymptotic state ϕ_+ in the distant future. To study such solutions one defines the Møller wave operators

$$W^\pm = s - \lim_{t\to\pm\infty} U(-t)U_0(t)P_{\mathrm{ac}}(H_0)\,. \tag{1.2}$$

Here $P_{\mathrm{ac}}(H_0)$ denotes the projection onto the subspace of absolute continuity of H_0. Assuming that the wave operators exist, one says that they are *asymptotically complete* if the ranges of W^+ and W^-, denoted $\operatorname{Ran} W^\pm$, coincide with the subspace of continuity of H, denoted $\mathcal{H}_{\mathrm{c}}(H)$. If the ranges of $W^\pm$ equal the subspace of absolute continuity of H, then the wave operators are said to be *strongly complete*; in other words, the singular continuous spectrum of H is empty. In that case the absolutely continuous parts of H_0 and H are unitarily equivalent via the wave operators. When the wave operators exist, one can define the scattering operator S in terms of the wave operators by the relation $S = (W^+)^*W^-$. The only nonzero matrix elements of the corresponding S-matrix are the diagonal scattering channel elements. The wave operators and the scattering operator are basic quantities in the mathematical description of the scattering process [21]. The S operator is a unitary operator in the scattering channel if and only if $\operatorname{Ran} W^+ = \operatorname{Ran} W^-$.

Within the context of QWs we compare L (the "perturbed" QW Hamiltonian) and the "free" Hamiltonian L_0 which is just the Dirichlet Laplacian associated with a straight QW. Imposing suitable conditions on the geometrical characteristics of the bend wire we will prove certain general properties of scattering in such semi-open structures. The main result asserts that the Møller wave operators exist and are strongly asymptotically complete. A state-of-the-art version of the celebrated Mourre method is used to derive the results.

The paper is organized as follows. We begin by demonstrating how Hamiltonians, describing the motion of quantum particles confined to semi-open, bend channels, can be expressed conveniently. For this purpose, in Section 2, we recall some basic facts about curves and frames. The QW Hamiltonians associated with straight and bend wires are introduced in Section 3 by means of sesquilinear forms. Their mathematical structure motivates the investigation of a fairly general class of Hamiltonians on cylindrical Lipschitz domains which is summarized in Sections 4, 5, and 6. For a pair of such Hamiltonians we prove existence and strong asymptotic completeness of their wave operators; see Theorem 6.3. The abstract results are based on a limiting absorption principle, established in [22], valid in a framework of weighted Sobolev spaces. In Section 7 we state our main results, which are applications of the abstract theory to QWs; see Theorems 7.2–7.3.

For related work, we refer to [23–30]. Discussions of (general) systems with constraints can be found in [31]. Quasi-bound states are discussed in [32–34]; in the latter the stationary approach is used. The role of impurity scattering is discussed in [35–40].

Having set the scene in this paper by establishing the basic scattering theory, we hope that physicists and applied mathematicians will be attracted to this exciting topic and pursue the study of scattering processes of QWs, *e.g.* local decay of wave functions, low-energy properties, quasi-bound states, eigenfunction expansions, appearence of quasi-bound states *etc.*

Finally, a few words about notation. We adopt the usual notation for function spaces: C_0^∞, L^2, *etc.* For a Lipschitz domain $\Omega \subset \mathbb{R}^d$ or, alternatively, a domain with a "boundary with minimal regularity" (see, *e.g.* [41]) the (local) Sobolev spaces $\boldsymbol{H}^s(\Omega)$ and $\boldsymbol{H}_0^s(\Omega)$ $(s \in \mathbb{R})$ have the standard properties. We adopt the standard notation of tensor calculus, we suppress sums over indices, and the symbol δ_{ij} refers to the components of the Euclidean metric matrix 1. Moreover, we shall freely use various notation for (partial) derivatives (*e.g.* dots, commas, ∂_j, and ∂^α with α being a multi-index).

2. Curves, frames, and wires

We summarize some facts about curves and frames which enable us to describe bend wires in a convenient way.

A (parametrized) *curve* in $\mathbb{R}^n$ is a C^∞ mapping $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$, $n \geq 2$. The curve $\boldsymbol{\alpha}$ is said to be *regular* provided $\dot{\boldsymbol{\alpha}}(\xi) \neq 0$ for all $\xi \in \mathbb{R}$. The variable ξ is called the *parameter* of the curve. The tangent space $\mathbb{R}_{\xi_0} = \boldsymbol{T}_{\xi_0}\mathbb{R}$ of $\mathbb{R}$ at $\xi_0 \in \mathbb{R}$ has a distinguished basis $1 = (\xi_0, 1)$. The differential of $\boldsymbol{\alpha}$ at ξ_0, $d\boldsymbol{\alpha}_{\xi_0}(1) \in \boldsymbol{T}_{\boldsymbol{\alpha}(\xi_0)}\mathbb{R}^n$, is well-defined and one has $d\boldsymbol{\alpha}_{\xi_0}(1) = \dot{\boldsymbol{\alpha}}(\xi_0)$; the derivative of the $\mathbb{R}^n$-valued function $\boldsymbol{\alpha}(\xi)$ at ξ_0.

A *vector field along* $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$ is a differentiable mapping $X : \mathbb{R} \to \mathbb{R}^n$. The vector field along $\boldsymbol{\alpha}$ given by $\xi \mapsto \dot{\boldsymbol{\alpha}}(\xi)$ is the *tangent vector field*. We think of $X(\xi)$, *i.e.* the value of X at a given $\xi \in \mathbb{R}$, as lying in the copy of $\mathbb{R}^n$ identified with $\boldsymbol{T}_{\boldsymbol{\alpha}(\xi)}\mathbb{R}^n$.

The curve $\boldsymbol{\alpha}(\xi)$ is said to be a *unit-speed* curve or *parameterized by arc length* if $|\dot{\boldsymbol{\alpha}}(\xi)| = 1$ for all $\xi \in \mathbb{R}$; any regular curve can be parametrized by arc length (see, *e.g.* [42]).

Definition 2.1. Let $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$, $n \geq 2$, be a curve.

(H1) A *moving n-frame along* $\boldsymbol{\alpha}$ is a family of differentiable mappings $\hat{e}_i : \mathbb{R} \to \mathbb{R}^n$, $1 \leq i \leq n$, such that for all $\xi \in \mathbb{R}$, $\hat{e}_i(\xi) \cdot \hat{e}_j(\xi) = \delta_{ij}$, where δ_{ij} is Kronecker's delta function. Each $\hat{e}_i(\xi)$ is a vector field along $\boldsymbol{\alpha}$, and $\hat{e}_i(\xi)$ is viewed as a vector in $\boldsymbol{T}_{\boldsymbol{\alpha}(\xi)}\mathbb{R}^n$.

(H2) A moving n-frame is said to be a *Frenet n-frame*, or merely a *Frenet frame*, if for all k, $1 \leq k \leq n$, the k-th derivative $\boldsymbol{\alpha}^{(k)}(\xi)$ of $\boldsymbol{\alpha}(\xi)$ lies in the span of the set $\{\hat{e}_1(\xi), \ldots, \hat{e}_n(\xi)\}$.

We recall (see, *e.g.* [42]):

Lemma 2.2. *Suppose* $\boldsymbol{\alpha} : \mathbb{R} \to \mathbb{R}^n$*,* $n \geq 2$*, is a curve such that the vectors* $\dot{\boldsymbol{\alpha}}(\xi), \boldsymbol{\alpha}^{(2)}(\xi), \ldots, \boldsymbol{\alpha}^{(n-1)}(\xi)$ *are linearly independent for all* ξ*. Then there exists a unique Frenet frame with the following properties*

• *For* $1 \leq k \leq n-1$*,* $\dot{\boldsymbol{\alpha}}(\xi), \boldsymbol{\alpha}^{(2)}(\xi), \ldots, \boldsymbol{\alpha}^{(k)}(\xi)$ *and* $\hat{e}_1(\xi), \ldots, \hat{e}_k(\xi)$ *have the same orientation.*

(H3) *The vectors* $\hat{e}_1(\xi), \ldots, \hat{e}_n(\xi)$ *have the positive orientation.*

A frame for which properties (H1)–(H3) hold, together with the first assertion in Lemma 2.2, is referred to as a *distinguished Frenet frame*. For dimensions $n \geq 3$ the first assertion of Lemma 2.2 rules out curves belonging to subspaces of lower dimension.

Henceforth we consider a regular unit-speed curve $\boldsymbol{\alpha}$ in association with a Frenet frame $\{\hat{e}_i(\xi)\}$, $1 \leq i \leq n$, $\xi \in \mathbb{R}$ such that the above-mentioned properties (H1)-(H3) hold, together with

(H4) $\hat{e}_1(\xi) = \dot{\boldsymbol{\alpha}}(\xi)$.

(H5) The vector $\dot{\hat{e}}_i(\xi)$ lies in the span of $\hat{e}_1(\xi), \ldots, \hat{e}_{i+1}(\xi)$.

Then we have:

Lemma 2.3. *Under the above-mentioned hypotheses (H1)–(H5), the Serret–Frenet formulae hold, i.e.,*

$$\dot{\hat{e}}_i = \Xi_i^j \hat{e}_j, \tag{2.1}$$

where $\Xi \equiv (\Xi_i^j)$ *is defined by*

$$\Xi := \begin{pmatrix} 0 & \kappa_1 & 0 & \cdots & 0 \\ -\kappa_1 & 0 & \kappa_2 & \cdots & 0 \\ \vdots & -\kappa_2 & \ddots & \ddots & \\ 0 & \cdots & -\kappa_{n-2} & 0 & \kappa_{n-1} \\ 0 & \cdots & & -\kappa_{n-1} & 0 \end{pmatrix}. \tag{2.2}$$

The $n \times n$ matrix Ξ is skew-symmetric and the functions

$$\kappa_i(\xi) = \dot{\hat{e}}_i(\xi) \cdot \hat{e}_{i+1}(\xi), \quad i = 1, \ldots, n-1; \tag{2.3}$$

are positive and smooth with respect to the parameter ξ.

A standard result in the theory of ordinary differential equations (see, *e.g.* [43]) gives us the following result.

Lemma 2.4. *Let the above-mentioned hypotheses (H1)–(H5) be fulfilled. Then the initial value problem*

$$\dot{\Theta}_i^j + \Theta_i^r \Xi_r^j = 0\,, \tag{2.4}$$

$$\delta_{rs}\Theta_i^r(\xi_0)\Theta_j^s(\xi_0) = \delta_{ij} \text{ and } \det(\Theta_i^j(\xi_0)) = 1 \tag{2.5}$$

has a unique C^∞ solution on $\mathbb{R}$.

The initial condition (2.5) means that the matrix $(\Theta_{\mathrm{i}}^j(\xi_0))$ is a rotation matrix in $\mathbb{R}^{n-1}$ for $\xi_0 \in \mathbb{R}$. Introduce

$$\Theta := (\Theta_i^j) = \begin{pmatrix} 1 & 0 \\ 0 & (\Theta_r^s) \end{pmatrix}.$$

Lemma 2.4 justifies the definition of the following moving frame $e_1, \ldots, e_n$ along $\boldsymbol{\alpha}$:

$$e_i := \Theta_i^j \hat{e}_j\,. \tag{2.6}$$

Having chosen the latter frame, we may proceed to wires. Let $B_r \subset \mathbb{R}^{n-1}$ denote the open ball centered at the origin and having radius $r > 0$. Introduce the straight wire $T := \mathbb{R} \times B_r$ and define the bend wire $\mathcal{T}$ of radius r about $\boldsymbol{\alpha}$ by means of the map $\Gamma : \mathrm{T} \to \mathbb{R}^n$ given as

$$(\xi, \eta^2, \ldots, \eta^n) \mapsto \boldsymbol{\alpha}(\xi) + e_i(\xi)\eta^i\,. \tag{2.7}$$

The Serret–Frenet equations (2.1) in conjunction with (2.5) imply that

$$\dot{e}_1 = \kappa_1 \hat{e}_2 \text{ and } \dot{e}_i = \Theta_i^j \Xi_j^1 \hat{e}_1 = -\kappa_1 \Theta_i^2 \hat{e}_1\,. \tag{2.8}$$

The implicit function theorem ensures that the map $\Gamma : \mathrm{T} \to \mathcal{T}$ is a local diffeomorphism provided $\kappa_1 \in L^\infty(\mathbb{R})$ and $r\|\kappa_1\|_{L^\infty(\mathbb{R})} < 1$. The diffeomorphism becomes global if $\mathcal{T}$ does not intersect itself. Henceforth we shall thus impose the following constraints:

Assumption 2.5.

(i) Regularity at infinity: $\kappa_1 \in L^\infty(\mathbb{R})$.

(ii) Restriction on radius of B_r: $r\|\kappa_1\|_{L^\infty(\mathbb{R})} < 1$.

(iii) $\mathcal{T}$ does not intersect itself.

In particular, a system of global co-ordinates (ξ, η), $\eta := (\eta^2, \ldots, \eta^n)$ is determined by the inverse map Γ^{-1}.

3. Model of quantum wires

The following set-up is standard [8, 11, 44]. Let $\mathbb{R} \ni \xi \mapsto \boldsymbol{\alpha}(\xi)$ be a C^∞, unit-speed curve in $\mathbb{R}^n$, $n \geq 2$. With respect to the Frenet frame in (2.6) its i^{th} curvature is given by $\kappa_i(\xi)$, $i = 1, \ldots, n-1$, in (2.3). The bend wire $\mathcal{T}$ will be identified with

$$\mathcal{T} = \{\, x \in \mathbb{R}^n \,:\, \operatorname{dist}(x, \boldsymbol{\alpha}) < r \,\} \tag{3.1}$$

for some $r > 0$; *cf.* (2.7). Henceforth we impose Assumption 2.5.

The motion of a quantum particle confined to the wire $\mathcal{T}$ depends on its interaction with the boundary, denoted $\partial\mathcal{T}$, of $\mathcal{T}$. Throughout we consider the Dirichlet Laplacian $-\Delta_{D,\mathcal{T}}$, *i.e.*, the Friedrichs extension of the map $\psi \mapsto -\Delta\psi$ defined on $C_0^\infty(\mathcal{T})$; this corresponds to infinitely hard walls at $\partial\mathcal{T}$.

Below we shall rigorously introduce the QW Hamiltonians associated with a straight wire and the bend wire given in (3.1).

"Free" QW. On $L^2(T)$ we consider the sesquilinear form $\mathfrak{l}_0$ with domain $\mathfrak{Q}(\mathfrak{l}_0) = \boldsymbol{H}_0^1(T)$ defined by

$$\mathfrak{l}_0[u, v] := \langle u_{,i}, \delta^{ij} v_{,j} \rangle_{L^2(\mathrm{T})}, \quad u, v \in \boldsymbol{H}_0^1(T)\,. \tag{3.2}$$

It is a densely defined, symmetric, non-negative closed form. A form core of $\mathfrak{l}_0$ is $C_0^\infty(T)$. Kato's representation theorem [41, Theorem VI.2.4] gives a unique Hamiltonian[1] L_0 in $L^2(T)$ with domain

$$\begin{aligned} \mathfrak{D}(L_0) :\; &= \big\{\, v \in \boldsymbol{H}_0^1(T) \,:\, \exists u \in L^2(T) \text{ such that} \\ \mathfrak{l}_0[v, \varphi] \;&=\; \langle u, \varphi \rangle_{L^2(T)} \quad \forall \varphi \in \boldsymbol{H}_0^1(T)\,. \end{aligned} \tag{3.3}$$

We have

$$\mathfrak{D}(L_0) \;=\; \{\, u \in \boldsymbol{H}_0^1(T) \,:\, \Delta u \in L^2(T) \,\} \tag{3.4}$$

$$L_0 u \;=\; -\Delta u \quad \text{if} \quad u \in \mathfrak{D}(L_0)\,. \tag{3.5}$$

The Dirichlet Laplacian $-\Delta_{D,B_r}$ on $L^2(B_r)$ generated by the sesquilinear form

$$\mathfrak{q}[u, v] := \langle u_{,i}, \delta^{ij} v_{,j} \rangle, \quad u, v \in \boldsymbol{H}_0^1(B_r)\,, \tag{3.6}$$

has purely discrete spectrum consisting of energies $(0 <)\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots$. The latter constitutes the threshold set $\mathit{\Lambda} := \{\lambda_n \,:\, n \in \mathbb{N}\}$. The unperturbed Hamiltonian L_0 clearly has the tensor decomposition $L_0 = -\partial_\xi^2 \otimes I + I \otimes -\Delta_{D,B_r}$. Moreover, one has $\sigma(L_0) = \sigma_{\text{ess}}(L_0) = [\lambda_1, \infty)$.

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[1] *i.e.* a self-adjoint operator.

"Perturbed" QW. The bend wire $\mathcal{T}$ can be identified with a Riemannian manifold (T, m) with $m := (m_{ij})$ being the metric generated from (2.7). Evidently, $m_{ij} := \Gamma_{,i} \cdot \Gamma_{,j}$ and, due to (2.8), we have that

$$m = \operatorname{diag}(l^2, 1, \ldots, 1) \quad \text{where} \quad l(\xi, \eta) := 1 + \eta^i \Theta_i^j \Xi_j^1. \tag{3.7}$$

Denoting by $d\eta$ the $(n-1)$-dimensional Lebesgue measure in B_r, a volume element of $\mathcal{T}$ is defined via $d\tau := l(\xi, \eta)\, d\xi d\eta$ because $|m| := \det m = l^2$. To obtain a unique self-adjoint realization of the Dirichlet Laplacian $-\Delta_{D,\mathcal{T}}$ in $L^2(\mathcal{T})$, we set $(m^{ij}) := m^{-1}$ and define a sesquilinear form $\widetilde{\mathfrak{l}}$ with domain $\mathfrak{Q}(\widetilde{\mathfrak{l}}) = \boldsymbol{H}_0^1(\mathrm{T}, d\tau)$ by $\widetilde{\mathfrak{l}}[u,v] := \langle u_{,i}, m^{ij} v_{,j} \rangle_{L^2(T, d\tau)}$, for $u, v \in \mathfrak{Q}(\widetilde{\mathfrak{l}})$. It is clearly densely defined, symmetric, non-negative and closed on $\mathfrak{Q}(\widetilde{\mathfrak{l}})$. Invoking once again Kato's representation theorem, we get a unique non-negative Hamiltonian $\widetilde{L}$ satisfying $\mathfrak{D}(\widetilde{L}) \subset \mathfrak{Q}(\widetilde{\mathfrak{l}})$ and $\widetilde{\mathfrak{l}}[u,v] = \langle u, \widetilde{L} v \rangle_{L^2(\mathrm{T}, d\tau)}$ for $u \in \mathfrak{Q}(\widetilde{\mathfrak{l}}),\ v \in \mathfrak{D}(\widetilde{L})$. For any element

$$u \in \mathfrak{D}(\widetilde{L}) := \{\, v \in \boldsymbol{H}_0^1(T, d\tau) \,:\, \partial_i |m|^{\frac{1}{2}} m^{ij} \partial_j v \in L^2(T, d\tau) \,\}$$

one has

$$\widetilde{L} u = -|m|^{-\frac{1}{2}} \partial_i |m|^{\frac{1}{2}} m^{ij} \partial_j u\,.$$

In other words, $\widetilde{L}$ equals the Dirichlet Laplacian $-\Delta_{D,\mathcal{T}}$ expressed by means of the co-ordinates (ξ, η), $\eta = (\eta^2, \ldots, \eta^n)$.

Transformation to flat boundary. It is advantageous to transform the wire to a flat boundary which is possible under Assumption 2.5. Indeed, the Hamiltonian $\widetilde{L}$ can be transformed into a unitarily equivalent operator L of the form

$$L = -\partial_i m^{ij} \partial_j + V_{\text{bend}} \tag{3.8}$$

acting in $L^2(T)$. In particular, we get rid of the weight $|\mathrm{m}|^{\frac{1}{2}}$ in the volume element. This trick of "flattening" goes back to [45] (in a different physical context). For this purpose we introduce the unitary operator $U : L^2(T, d\tau) \to L^2(T)$ defined by $u \mapsto |\mathrm{m}|^{\frac{1}{4}} u$. Setting $L := U \widetilde{L} U^{-1}$, we obtain

$$\begin{aligned} Lu &= -|m|^{-\frac{1}{4}} \partial_i |m|^{\frac{1}{2}} \mathrm{m}^{ij} \partial_j |m|^{-\frac{1}{4}} u, \qquad \text{for} \\ u \in \mathfrak{D}(L) &= \{ u \in \boldsymbol{H}_0^1(T) \,:\, \partial_i |m|^{\frac{1}{2}} m^{ij} \partial_j |\mathrm{m}|^{-\frac{1}{4}} u \in L^2(T) \,\}\,. \end{aligned}$$

By commutating the first order differential operators appearing in L with $m^{-\frac{1}{4}}$ and inserting the original expression for m, we derive (3.8) with

$$V_{\text{bend}} := -\frac{5}{4} \frac{(l_{,1})^2}{l^4} + \frac{1}{2} \frac{l_{,11}}{l^3} - \frac{1}{4} \frac{\delta^{ij} l_{,i} l_{,j}}{l^2} + \frac{1}{2} \frac{\delta^{ij} l_{,\mathrm{ij}}}{l}\,. \tag{3.9}$$

4. Abstract Hamiltonian on a cylindrical domain

Instead of working directly with L and L_0, the Hamiltonians for the QWs, we shall study two abstract Hamiltonians A and A_0 defined on a cylindrical Lipschitz domain $\mathcal{M} = \mathbb{R} \times Q$, where $Q \subset \mathbb{R}^{n-1}$, $n \geq 2$, is an open and bounded Lipschitz domain. Specifically, A and A_0 act as follows

$$A = -\partial_i m^{ij} \partial_j + V \text{ and } A_0 = -\partial_i \delta^{ij} \partial_j \tag{4.1}$$

on $L^2(\mathcal{M})$ with Dirichlet boundary conditions; as usual sums over indices are suppressed. The structure of A is motivated by the discussion in Section 3 and the expression (3.8). The matrix-valued function $M \equiv (m^{ij})$ is real-valued and symmetric on $\mathcal{M}$ and V is a multiplication operator induced by a real-valued function on $\mathcal{M}$. In the sequel $x = (x_1, \tilde{x})$ is a vector of $\mathbb{R} \times Q$ and $\langle x \rangle := (1 + |x|^2)^{\frac{1}{2}}$ for $x \in \mathcal{M}$. We shall impose the following conditions on M and V.

Assumption 4.1. The following inequalities are understood in the sense of matrices.

(i) There exist positive constants c and C such that

$$c \leq M(x) \leq C \text{ for a.e. } x \in \mathcal{M}.$$

(ii) There exists $\mu_1 > 1$ and a positive constant C_1 such that $v^{ij}(x) := m^{ij} - \delta^{ij}(x)$ satisfies

$$|v^{ij}(x)| \leq C_1 \langle x_1 \rangle^{-\mu_1} \text{ for a.e. } x \in \mathcal{M}.$$

(iii) There exists $\mu_2 > 1$ and a positive constant C_2 such that

$$|\partial_1 m^{ij}(x)| \leq C_2 \langle x_1 \rangle^{-\mu_2} \text{ for a.e. } x \in \mathcal{M}.$$

In particular, Assumption 4.1*(ii)* implies that

(ii)'

$$\lim_{d \to \infty} \|\chi(\pm x_1 \geq d)(m^{ij}(x) - \delta^{ij})\|_{L^\infty(\mathcal{M})} = 0 \quad \forall i, j = 1, \ldots, n.$$

Assumption 4.2.

(i) Let $V \in L^\infty(\mathcal{M})$.

(ii) There exists $\nu_1 > 1$ and a positive constant C_3 such that

$$|V(x)| \leq C_3 \langle x_1 \rangle^{-\nu_1} \text{ for a.e. } x \in \mathcal{M}.$$

(iii) There exists $\nu_2 > 1$ and a positive constant C_4 such that

$$|\partial_1 V(x)| \leq C_4 \langle x_1 \rangle^{-\nu_2} \text{ for a.e. } x \in \mathcal{M}.$$

In particular, Assumption 4.2*(ii)* implies that
(ii)'

$$\lim_{d\to\infty} \|\chi(\pm x_1 \geq d)\, V(x)\|_{L^\infty(\mathcal{M})} = 0\,.$$

We then introduce the sesquilinear form $\widetilde{\mathfrak{a}}$ with domain $\boldsymbol{H}^1_0(\mathcal{M})\times\boldsymbol{H}^1_0(\mathcal{M})$ defined by $\widetilde{\mathfrak{a}}[\varphi,\psi] = \langle \partial_i\varphi, m^{ij}\partial_j\psi\rangle$ for $\varphi,\psi \in \boldsymbol{H}^1_0(\mathcal{M})$. It is clearly densely defined and symmetric. In view of Assumption 4.1 the matrix M is bounded and uniformly positive and, consequently, the form $\widetilde{\mathfrak{a}}$ is non-negative and closed. Invoking Kato's representation theorem, we get an unique Hamiltonian $\widetilde{A}$. Since, moreover, Assumption 4.2 ensures that V is bounded, the KLMN theorem [46, Theorem X.17] asserts that the sesquilinear form sum

$$\mathfrak{a}[\varphi,\psi] := \widetilde{\mathfrak{a}}[\varphi,\psi] + \langle \varphi, V\psi\rangle, \quad \varphi,\psi \in \mathfrak{Q}(\mathfrak{a}) = \mathfrak{Q}(\widetilde{\mathfrak{a}}) = \boldsymbol{H}^1_0(\mathcal{M})\,, \tag{4.2}$$

is closed and semi-bounded from below and hence it generates a Hamiltonian A.

5. Limiting absorption principle

The following spectral properties and limiting absorption principle (LAP) of A were obtained in [22]; the main result being the LAP. In very general terms, the LAP can be stated as follows for a self-adjoint operator T in a separable Hilbert space $\mathcal{H}$. Let $R(\zeta) = (T-\zeta)^{-1}$, $\operatorname{Im}\zeta \neq 0$, be the resolvent operator and let $\mathcal{X},\mathcal{Y}$ be Hilbert spaces such that $\mathcal{X}$ is densely and continuously embedded in $\mathcal{H}$ (and thus have a stronger norm). Then one says that T satisfies the LAP in an open set $\mathit{\Lambda} \subset \mathbb{R}$ if the limits

$$R^\pm(\lambda) = \lim_{\epsilon\to 0^+} R(\lambda \pm i\epsilon)\,, \quad \lambda \in \mathit{\Lambda}\,,$$

exist in the norm topology of $\mathcal{B}(\mathcal{X},\mathcal{Y})$, the space of bounded operators from $\mathcal{X}$ into $\mathcal{Y}$. The importance of the LAP lies in the fact that it implies some significant spectral properties of T (e.g, if a dense subset of $\mathcal{H}$ can be identified with elements of the dual space $\mathcal{Y}^*$ then T is absolute continuous in $\mathit{\Lambda}$). Furthermore, the LAP is an efficient tool to establish the scattering theory of T, as we demonstrate below.

The key ingredient in the proof of strong asymptotic completeness is a LAP valid in a framework of weighted Sobolev spaces $\boldsymbol{H}^s_{(\gamma)}(\mathcal{M}) := \{\psi \in \mathcal{D}'(\mathcal{M}) : \langle x\rangle^\gamma\psi \in \boldsymbol{H}^s(\mathcal{M})\}$ equipped with its natural norm; here $\mathcal{D}'(\mathcal{M})$ denotes the space of distributions. Evidently, for any $\gamma \geq 0$, one has continuous embeddings $\boldsymbol{H}^{-1}_{(\gamma)}(\mathcal{M}) \subset \boldsymbol{H}^{-1}(\mathcal{M})$ and $\boldsymbol{H}^1_0(\mathcal{M}) \subset \boldsymbol{H}^1_{(-\gamma)}(\mathcal{M})$. This version of the LAP, suitable for the study of scattering theory, is the content of assertion 4 in the following theorem, wherein $\mathit{\Upsilon}$ denote the set of eigenvalues of the Dirichlet Laplacian $-\Delta_{D,Q}$ on on the bounded Lipschitz domain Q in $\mathbb{R}^{n-1}$, $n \geq 2$.

Theorem 5.1. *Let $\mathcal{M}$, Q and Υ be as above. Suppose that the matrix M satisfies Assumption 4.1 (i), (ii)' and (iii) and that the potential V satisfies Assumption 4.2(i), (ii)' and (iii). Then the operator A in (4.1) has the following properties:*
1. The essential spectrum of A equals the semi-axis $[\upsilon_1, \infty)$ with $\upsilon_1 = \inf \Upsilon$.
2. The set of eigenvalues of A can accumulate only to the points of Υ and each eigenvalue away from Υ has finite multiplicity.
3. The operator A has no singular continuous spectrum.
4. For any $\gamma > 1/2$, the holomorphic functions

$$\mathbb{C}_\pm \ni \zeta \mapsto (A-\zeta)^{-1} \in \mathcal{B}(\boldsymbol{H}^{-1}_{(\gamma)}(\mathcal{M}), \boldsymbol{H}^{1}_{(-\gamma)}(\mathcal{M})) \tag{5.1}$$

extends continuously to $\mathbb{C}_\pm \cup (\mathbb{R} \setminus [\sigma_{\mathrm{p}}(A) \cup \Upsilon])$ in the uniform topology; here $\mathbb{C}_\pm := \{z \in \mathbb{C} : \pm \mathrm{Im}\, z > 0\}$.

Since Eidus' classic paper [47], the LAP has been extensively considered in spectral and scattering theory (see, *e.g.* [48, 49]). Although the proof of Theorem 5.1(4) follows a procedure well-known for the Laplace operator, the variable principle part of A requires a refined version of Mourre's method [50] within the context of pseudo-self-adjoint operators (see, *e.g.* [51]) and a substantially more complicated analysis of commutators. For further discussion and for a proof of Theorem 5.1 we refer to [22], wherein the reader also finds a list of related results.

6. Abstract result on scattering

We begin by introducing the "unperturbed" Hamiltonian A_0. On $L^2(\mathcal{M})$ we consider the sesquilinear form $\mathfrak{a}_0$ with domain $\mathfrak{Q}(\mathfrak{a}_0) = \boldsymbol{H}^1_0(\mathcal{M})$ defined by

$$\mathfrak{a}_0[\varphi, \psi] := \langle \partial_i \varphi, \delta^{ij} \partial_j \psi \rangle, \quad \varphi, \psi \in \boldsymbol{H}^1_0(\mathcal{M}). \tag{6.1}$$

It is a densely defined, symmetric, non-negative closed form. A form core of $\mathfrak{a}_0$ is $C_0^\infty(\mathcal{M})$. Kato's representation theorem gives a unique Hamiltonian A_0 in $L^2(\mathcal{M})$ with domain

$$\begin{aligned}\mathfrak{D}(A_0) := \{\, \psi \in \boldsymbol{H}^1_0(\mathcal{M}) \,:\, &\exists \varphi \in L^2(\mathcal{M}) \text{ such that} \\ &\mathfrak{a}_0[\psi, u] = \langle \varphi, u \rangle_{L^2(\mathcal{M})} \quad \forall u \in \boldsymbol{H}^1_0(\mathcal{M}) \,\}\,.\end{aligned} \tag{6.2}$$

We have

$$\mathfrak{D}(A_0) \;=\; \{\, \psi \in \boldsymbol{H}^1_0(\mathcal{M}) \,:\, \Delta\psi \in L^2(\mathcal{M}) \,\} \tag{6.3}$$

$$A_0 \psi \;=\; -\Delta \psi \quad \text{if} \quad \psi \in \mathfrak{D}(A_0). \tag{6.4}$$

The Dirichlet Laplacian $-\Delta_{D,Q}$ on $L^2(Q)$ generated by the sesquilinear form

$$\mathfrak{q}[\varphi, \psi] := \langle \partial_i \varphi, \delta^{ij} \partial_j \psi \rangle, \quad \varphi, \psi \in \boldsymbol{H}^1_0(Q), \tag{6.5}$$

has purely discrete spectrum consisting of eigenvalues $(0<)\upsilon_1<\upsilon_2\le\upsilon_3\le\cdots$. The latter constitute the threshold set $\Upsilon:=\{\upsilon_n : n\in\mathbb{N}\}$. The unperturbed Hamiltonian H_0 has the tensor decomposition $A_0=-\partial_1^2\otimes I+I\otimes-\Delta_{D,Q}$ and, furthermore, one has $\sigma(A_0)=\sigma_{\mathrm{ess}}(A_0)=[\upsilon_1,\infty)$.

We proceed to scattering theory for the pair (A,A_0). The following classic result goes back to Lavine [52].

Theorem 6.1. *Let T_1 and T_2 be two self-adjoint operators in a separable Hilbert space $\mathcal{H}$ with spectral projections $E_{T_1}(\Omega)$ and $E_{T_2}(\Omega)$. Assume that there exist sets Ω_j, $j\in\mathbb{N}$, and operators E_k, F_k, $1\le k\le N$, such that:*
(i) $\Omega=\cup_{j\in\mathbb{N}}\Omega_j$ where each Ω_j is a bounded open interval, and $\Omega_j\cap\Omega_k=\emptyset$ if $j\ne k$.
(ii) The operator E_k is T_1-bounded and locally T_1-smooth on Ω_j, for $1\le k\le N$, and $j\ge1$.
(iii) The operator F_k is T_2-bounded and locally T_2-smooth on Ω_j, for $1\le k\le N$, and $j\ge1$.
(iv) $T_2-T_1=\sum_{k=1}^N F_k^*E_k$ is valid in the sense of forms, i.e.

$$\langle T_2u,v\rangle_{\mathcal{H}}-\langle u,T_1v\rangle_{\mathcal{H}}=\sum_{k=1}^N\langle F_ku,E_kv\rangle_{\mathcal{H}},\quad u\in\mathfrak{D}(T_2),\ v\in\mathfrak{D}(T_1).$$

(v) Both sets $\sigma(T_1)\setminus\Omega$ and $\sigma(T_2)\setminus\Omega$ have Lebesgue measure zero.
Then the generalized wave operators

$$\begin{aligned}W^{\pm} &= s-\lim_{t\to\pm\infty}e^{itT_2}e^{-itT_1}P_{\mathrm{ac}}(T_1)\,,\\ \tilde{W}^{\pm} &= s-\lim_{t\to\pm\infty}e^{itT_1}e^{-itT_2}P_{\mathrm{ac}}(T_2)\end{aligned}$$

exist and are complete.

For our purpose, we choose $T_1=A_0$ and $T_2=A$ and $\Omega=\mathbb{R}\setminus\Upsilon$. For $u\in\mathfrak{D}(A)$ and $v\in\mathfrak{D}(A_0)$ we have

$$\begin{aligned}&\langle Au,v\rangle_{L^2(\mathcal{M})}-\langle u,A_0v\rangle_{L^2(\mathcal{M})}=\mathfrak{a}[u,v]-\overline{\mathfrak{a}}_0[v,u]\\&=\int_{\mathcal{M}}(\partial_iu)(x)v^{ij}\overline{(\partial_jv)(x)}\,dx\\&+\int_{\mathcal{M}}|V(x)|^{\frac12}u(x)|V(x)|^{\frac12}\operatorname{sign}V(x)\overline{v(x)}\,dx\,,\end{aligned}\tag{6.6}$$

where, on the right-hand side, we suppress the summations over i,j. Hence, by introducing the operators $E_{ij},F_{ij}:\boldsymbol{H}^1_{(-\gamma)}(\mathcal{M})\to L^2(\mathcal{M})$, $\gamma=\max\{\mu,\nu\}$, $1\le i,j\le n+1$, $\mu:=\max_{j=1,2}\mu_j/2$ (see Assumption 4.1 for the decay parameters μ_j), $\nu = \max_{j=1,2} \nu_j/4$ (see Assumption 4.2 for the decay parameters ν_j), defined by

$$\begin{aligned} E_{ij}u &:= \langle\cdot\rangle^{\mu} v^{ij}\partial_j u, \quad F_{ij}u := -\langle\cdot\rangle^{-\mu}\partial_i u \quad 1 \le i,j \le n\,, \\ E_{n+1}u &:= \langle\cdot\rangle^{\nu}|V|^{\frac{1}{2}}, \quad F_{n+1} = \langle\cdot\rangle^{-\nu}|V|^{\frac{1}{2}}\operatorname{sign} V\,, \end{aligned} \tag{6.7}$$

we have, in view of (6.6), that

$$A - A_0 = \sum_{1\le i,j\le n} F_{ij}^* E_{ij} + F_{n+1}^* E_{n+1} \tag{6.8}$$

holds in the sense of forms. In addition, we need the following auxiliary result.

Lemma 6.2. *Let $\gamma > 1/2$ and let $g \in L^\infty(\mathcal{M})$ be a function satisfying $\langle\cdot\rangle^\gamma g \in L^\infty(\mathcal{M})$. Then*
1. The operator $G : \boldsymbol{H}^1_{(-\gamma)}(\mathcal{M}) \to L^2(\mathcal{M})$, $Gu := g\partial^\alpha u$ (where α is a multi-index with order $|\alpha| \le 1$) is bounded.
2. The unbounded operator defined by G in $L^2(\mathcal{M})$, also denoted by G, is A-bounded.
3. The operator G is locally A-smooth on $\mathbb{R}\setminus\Upsilon$.

Proof. Evidently, the hypotheses on g and γ ensure that the first statement holds. The second statement follows from the inclusions $\mathfrak{D}(A) \subset \boldsymbol{H}^1_0(\mathcal{M}) \subset \boldsymbol{H}^1_{(-\gamma)}(\mathcal{M})$. To prove the third assertion we need to verify that for any compact set $K \subset \mathbb{R}\setminus\Upsilon$, the operator $GE_A(K)$ is A-smooth. A sufficient requirement for this is that (see, *e.g.* [48, Theorem XIII.30])

$$\sup_{\lambda\in K, 0<\epsilon<1} \|G(A-\lambda-i\epsilon)^{-1}G^*\|_{\mathcal{B}(L^2(\mathcal{M}))} < \infty\,. \tag{6.9}$$

From Theorem 5.1 we infer that

$$\sup_{\lambda\in K, 0<\epsilon<1} \|(A-\lambda-i\epsilon)^{-1}\|_{\mathcal{B}(\boldsymbol{H}^{-1}_{(\gamma)}(\mathcal{M}),\boldsymbol{H}^{1}_{(-\gamma)}(\mathcal{M}))} < \infty$$

and therefore (6.9) is fulfilled. This proves the third statement. □

We next recall the following notion. A real-valued function ϕ, defined on $\mathbb{R}_+$, is *admissible* provided

$$\lim_{t\to\infty} \int_0^\infty \left| \int_I e^{-it\phi(\lambda)-is\lambda}\, d\lambda \right|^2 ds = 0$$

for any bounded interval $I \subset \mathbb{R}_+$. Our main result is:

Theorem 6.3. *Let Assumption 4.1 and Assumption 4.2 be satisfied. Then*
1. The wave operators $W^{\pm} = s - \lim_{t\to\pm\infty} e^{itA}e^{-itA_0}$ *exist and are strongly asymptotically complete.*
2. If ϕ *is an admissible function, then* $W^{\pm} = s - \lim_{t\to\pm\infty} e^{it\phi(A)}e^{-it\phi(A_0)}$.

Proof. It follows immediately from the discussion above, Theorem 5.1, Lemma 6.2 and Theorem 6.1. □

Related results are found in [53], also being based upon a variant of Mourre's method.

7. Main results for quantum wires

Herein we establish the main results on QWs by carrying over the abstract results on Hamiltonians of the type (4.1) to the QW Hamiltonians L_0 and L. We impose the following decay conditions on the curvatures.

Assumption 7.1.
(i) $\Xi_r^1(\xi), \ddot{\Xi}_r^1(\xi) \longrightarrow 0$ as $|\xi| \to \infty$ for $r = 2, \dots, n$.
(i)' There exists $\alpha > 1$ such that $\Xi_r^1(\xi), \ddot{\Xi}_r^1(\xi) = O\left(|\xi|^{-\alpha}\right)$ for $r = 2, \dots, n$.
(ii) $\Xi_r^s, \dot{\Xi}_r^2 \in L^\infty(\mathbb{R})$ for $r, s = 2, \dots, n$.
(iii) There exists $\beta > 1$ such that

$$\dot{\Xi}_r^1(\xi), \dddot{\Xi}_r^1(\xi), \Xi_r^2(\xi), \ddot{\Xi}_r^2(\xi), (\dot{\Xi}_r^s \Xi_s^2)(\xi), (\Xi_r^s \dot{\Xi}_s^2)(\xi) = O\left(|\xi|^{-\beta}\right)$$

for $r = 2, \dots, n$.
Our main results are the following two theorems. The first theorem states the basic spectral properties of L and, most importantly for scattering theory, it states the LAP for L in a framework of weighted Sobolev spaces.

Theorem 7.2. *Let Assumption 2.5 and Assumption 7.1(i), (ii) and (iii) be satisfied. Then*
1. The essential spectrum of L *equals the semi-axis* $[\lambda_1, \infty)$ *with* $\lambda_1 = \inf \Lambda$.
2. The set of eigenvalues of L *can accumulate only to the points of* Λ *and each eigenvalue away from* Λ *has finite multiplicity.*
3. The operator L *has no singular continuous spectrum.*
4. For any $\gamma > 1/2$, *the holomorphic functions*

$$\mathbb{C}_\pm \ni \zeta \mapsto (L-\zeta)^{-1} \in \mathcal{B}\left(\boldsymbol{H}^{-1}_{(\gamma)}(\mathcal{T}), \boldsymbol{H}^{1}_{(-\gamma)}(\mathcal{T})\right) \tag{7.1}$$

extends continuously to $\mathbb{C}_\pm \cup (\mathbb{R} \setminus [\sigma_{\mathrm{p}}(L) \cup \Lambda])$ *in the uniform topology.*

Theorem 7.2*(i)–(iii)* first appeared in [44]. The second result is the main contribution on scattering theory for the class of QWs which we consider:

Theorem 7.3. *Let Assumption 2.5 and Assumption 7.1(i)', (ii) and (iii) be satisfied. Then*
1. The wave operators $W^{\pm} = s - \lim_{t\to\pm\infty} e^{itL}e^{-itL_0}$ *exist and are strongly asymptotically complete.*
2. If ϕ *is an admissible function, then* $W^{\pm} = s - \lim_{t\to\pm\infty} e^{it\phi(L)}e^{-it\phi(L_0)}$.

Proofs of Theorems 7.2–7.3. Bear in mind the expressions for L in (3.8) and the one for V_{bend} in (3.9). In view of our abstract results, the proofs amount to translating Assumption 4.1 and Assumption 4.2 into conditions on the curvatures. By invoking the expression for l in (3.7), we get from (2.5) that

$$l_{,ij} = 0, \quad \delta^{ij} l_{,i} l_{,j} = \delta^{rs} \Xi_r^{\ 1} \Xi_s^{\ 1},$$

and an application of (2.4) yields

$$\begin{aligned} l_{,1}(\cdot,\eta) &= \eta^i \Theta_i^r \left(\dot{\Xi}_r^{\ 1} - \Xi_r^{\ s} \Xi_{\text{s}}^{\ 1} \right), \\ l_{,11}(\cdot,\eta) &= \eta^i \Theta_i^{\text{r}} \left(\ddot{\Xi}_r^{\ 1} - \Xi_r^{\ s} \Xi_s^{\ 1} - 2\Xi_r^{\ s} \dot{\Xi}_s^{\ 1} + \Xi_r^{\ s} \Xi_{\text{s}}^{\ t} \Xi_t^{\ 1} \right). \end{aligned}$$

In this way we have all terms appearing in V_{bend}. In view of Assumption 4.2 we must also compute

$$\begin{aligned} (V_{\text{bend}})_{,1} &= 5\frac{(l_{,1})^3}{l^5} - 4\frac{l_{,1}l_{,11}}{l^4} + \frac{l_{,111}}{2l^3} \\ &\quad + \frac{\delta^{ij}}{2}\left[\frac{l_{,1}l_{,i}l_{,j}}{l^3} - \frac{l_{,1}l_{,ij} + l_{,1\text{i}}l_{,j}}{l^2} + \frac{l_{,1ij}}{l} \right]. \end{aligned}$$

wherein

$$\begin{aligned} l_{,1ij} &= 0, \quad (\delta^{ij} l_{,i} l_{,j})_{,1} = 2\delta^{rs} \dot{\Xi}_r^{\ 1} \Xi_s^{\ 1}, \\ l_{,111}(\cdot,\eta) &= \eta^i \Theta_i^r \Big(\dddot{\Xi}_r^{\ 1} - 3\dot{\Xi}_r^{\ s} \dot{\Xi}_r^{\ 1} - 3\Xi_r^{\ \text{s}} \ddot{\Xi}_s^{\ 1} - \ddot{\Xi}_r^{\ s} \Xi_s^{\ 1} \\ &\qquad + \dot{\Xi}_r^{\ s} \Xi_s^{\ \text{t}} \Xi_t^{\ 1} + 2\Xi_r^{\ s} \dot{\Xi}_s^{\ t} \Xi_t^{\ 1} + 3\Xi_r^{\ s} \Xi_s^{\ t} \dot{\Xi}_t^{\ 1} - \Xi_r^{\ s} \Xi_s^{\ t} \Xi_t^{\ u} \Xi_u^{\ 1} \Big). \end{aligned}$$

From here on it remains to check that the conditions imposed in Assumption 4.1 and Assumption 4.2 give the ones formulated in Assumption 7.1. Using that $|\eta^j \Theta_j^s| < r$ (r being the radius of $\mathcal{T}$), this is rather easy to check. □

It is instructive to formulate the results in the two-dimensional case.

Theorem 7.4. *Suppose* $n = 2$ *and let Assumption 2.5 be satisfied.*
1. If $\kappa(\xi), \ddot{\kappa}(\xi) \to 0$ *as* $|\xi| \to \infty$ *and there exists* $\alpha > 1$ *such that* $\dot{\kappa}(\xi), \dddot{\kappa}(\xi) = O(|\xi|^{-\alpha})$, *then the assertions of Theorem 7.2 hold.*

2. If there exists $\beta > 1$ such that $\kappa(\xi), \dot{\kappa}(\xi), \ddot{\kappa}(\xi), \dddot{\kappa}(\xi) = O(|\xi|^{-\beta})$, then the assertions of Theorem 7.3 hold.

In two dimensions strong asymptotic completeness and $\sigma_{\rm sc}(L) = \emptyset$ were established by *stationary* scattering theory by Duclos *et al.* [24] provided $\kappa(\xi), \dot{\kappa}(\xi)^2, \ddot{\kappa}(\xi) = O(|\xi|^{-(1+\epsilon)})$. A similar result in two dimensions, under the same assumptions, was recently established by Melgaard [30] using a hybrid of the *time-dependent* Enss–Mourre method [23, 50]; a slightly different spectral result is obtained as a result of the method. Comparing the latter results with the ones herein, the results ($\sigma_{\rm sc}(L) = \emptyset$ and LAP) of Theorem 7.4(1) demand a stronger decay condition on $\dot{\kappa}$ and requires that $\dddot{\kappa}$ decays as $O(|\xi|^{-\alpha})$ at infinity for $\alpha > 1$. On the other hand, Theorem 7.4(1) requires much slower decay on κ and $\ddot{\kappa}$ compared to the afore-mentioned results. As for asymptotic completeness, the results of Theorem 7.4(2) require a weaker decay condition on $\dot{\kappa}$ and that $\dddot{\kappa}$ decays as $O(|\xi|^{-\beta})$ at infinity for $\beta > 1$.

8. Conclusions and perspectives

A rigorous treatment of the basic scattering properties of a nanoparticle moving in a narrow, bend channel (a so-called quantum wire) is developed by means of abstract results for a Hamiltonian considered on a cylindrical Lipschitz domain. Under certain general restrictions on the geometry of the wire, expressed in terms of the curvature, the following properties are established: (1) The Møller wave operators exist and the S operator is unitary in the scattering channels. (2) The singular continuous spectrum is empty. These properties underpin much of the existing literature on scattering and transmission processes for such mesoscopic systems and set the stage for future work on related issues (*e.g.* local decay of wave functions, low-energy scattering, quasi-bound states *etc*).

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