ELECTRICAL CONDUCTIVITY AND SCATTERING MATRIX FOR DIRAC OPERATORS ON MANIFOLDS WITH CYLINDRICAL CONTACTS

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Abstract. In the static limit of linear response theory, the electrical conductivity is a linear operator taking closed electric fields into closed electric current densities. The induced mapping in cohomology is called the electrical conductance. Using the notion of relative de Rham cohomology of a manifold M with boundary, we give a thorough discussion of what is meant by the transport part of the conductance of an open mesoscopic system.

We then consider the quantum mechanical setting of a generalized Dirac operator D acting on the sections of a Hermitian vector bundle over a Riemannian manifold M with cylindrical ends. The Kubo formula of linear response theory gives us an expression for the electrical conductivity in terms the resolvent kernel of D. Building on results from mathematical scattering theory, we prove that the Kubo formula is equivalent to the Landauer-Büttiker formula expressing the electrical conductance in terms of scattering data of the generalized Dirac operator. This is a rigorous version of an argument made by Baranger and Stone for the case of magnetic Schrödinger operators.

1. Introduction

The current response of an electrical conductor under standard conditions, say one volt per meter applied to a millimeter size copper cable at room temperature, is ruled approximately by Ohm's law. Valid in the classical limit of charge carriers with dissipative dynamics, this law in its local formulation relates the current density j to the electric field E. For a homogeneous isotropic material with electrical conductivity σ, Ohm's law in the static limit says that $j = \sigma \star E$ where $\star$ is the Hodge star operator (taking the 1-form E to the twisted 2-form j).

In a sub-micron size conductor at sub-Kelvin temperatures and zero voltage bias, the processes of electric charge transport want treatment in a quantum-theoretic framework. In fact, under such 'mesoscopic' conditions the electron motion is close to being dissipationless, phase coherence of the electron wave function is maintained over length scales greater than the system size, and the relation between E and j becomes nonlocal. The electrical conductivity, which in Ohm's case was just a number, now is a kernel (of the type of a bi-vector field) giving the current response in the static, or d.c., limit as an integral: $j^i(x) = \int \sigma^{ii'}(x,x')E_{i'}(x')d^dx'$.

Assuming the noninteracting electron approximation, Baranger and Stone [1] have made a detailed analysis of the d.c. linear current response for the case of magnetic Schrödinger operators, i.e., spinless nonrelativistic charged particles moving in a static electromagnetic field and in the mean field due to the other particles. They demonstrated (see also a related paper by M. Janssen [8]) that the standard Kubo-Greenwood theory of d.c. linear current response is equivalent to the scattering-theoretic approach of Landauer as reformulated by Büttiker.

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An important message from [1] in this context is the necessity to distinguish the electrical conductivity from the electrical *conductance*. The d.c. linear response conductivity is a linear operator taking rotationless electric fields E to divergenceless current densities j. Conductance, on the other hand, is the induced map in *cohomology*, sending the cohomology class of E, namely the electrical voltage $V := [E]$, to the electrical current $I := [j]$. While the conductivity receives contributions from electron states of all energies in general, the zero temperature limit of the conductance is determined by Green's functions at the Fermi energy ε_F alone. It is the transport part of the latter which admits a Landauer-Büttiker formula in terms of the on-shell scattering matrix evaluated at ε_F.

While the analysis of [1] was carried out for the case of electrons with magnetic Schrödinger dynamics, the physical situation may sometimes call for a different description of the charge carrier dynamics. Relevant examples that have received much attention of late are graphene, i.e., two-dimensional graphite, and its cylindrical cousins, the so-called carbon nanotubes. In these systems the low-energy effective dynamics is governed by a first-order operator of Dirac type. In the present paper we revisit the analysis of Baranger and Stone for such cases.

Our treatment is based on a d-dimensional compact Riemannian manifold M modelling the mesoscopic conductor. M is chosen to have a boundary $\partial M =: Y$, and we attach cylindrical ends $\mathbb{R}_+ \times Y$ to it to build the configuration manifold $X := M \cup_{\partial M} (\mathbb{R}_+ \times Y)$ of our open quantum system. The quantum dynamics is generated by a first-order differential operator D of Dirac type acting on the sections of a Hermitian vector bundle over X. We make the important assumption of translation invariant dynamics on $\mathbb{R}_+ \times Y$ (called 'perfectly conducting leads' in the physics literature), which is to ensure that

(1) the electrical conduction properties of (X, D) are determined by the mesoscopic conductor, i.e., by (M, D) and not by the measuring device $\mathbb{R}_+ \times Y$;
(2) we can set up a scattering-theoretic formalism for the problem;
(3) it is consistent and plausible on physical grounds to make the further assumption that the electric field strength E vanishes far out in the leads.

In this concise setting, our goal is to achieve a rigorous understanding of the relation between the formulas of Kubo and Landauer-Büttiker.

The paper begins, in Sect. 2, with a summary of some basic facts of cohomology underlying electrical transport theory in the d.c. linear response limit. While the electrical current $I = [j]$ naturally fits into the scheme of twisted de Rham cohomology (twisting being done by the orientation line bundle L of X), the proper notion to use in the case of the electrical voltage $V = [E]$ is cohomology with compact supports. In this context we recall that there is a nondegenerate pairing between currents $I \in H^{d-1}(X; L)$ and voltages $V \in H^1_c(X)$ by Poincaré duality. Using the notion of relative de Rham cohomology of a manifold with boundary, we show how to eliminate ring voltages and loop currents from the formalism and give a precise definition of what is meant by the *transport* part of the conductance.

In Sect. 3 we expand our considerations based on classical electrostatics by the framework of quantum theory for charged particles. For the case of a Hermitian vector bundle $E \to X$ with connection ∇, we construct the current operator J associated to a differential operator D_∇ by the principle of minimal substitution $D_\nabla \to D_{\nabla + A}$ with gauge field A. Transcribing this construction to the case of kernels, we write down the Kubo formula for the bi-vector field of the electrical conductivity as a current-current correlation function.

The heart of the paper is Sect. 4, where we set up the scattering formalism for (X, D). To do so in a satisfactory manner, we make use of a variant of scattering theory that applies to the case where the full Hamiltonian D acts in a Hilbert space which is different from that of the free Hamiltonian D_0. (In our case D_0 is D restricted to the cyclindrical ends with suitable boundary conditions.) We analytically continue the free scattering states to a Riemann surface constructed from the spectral data of D_0. Drawing on work by Guillopé [6] and W. Müller [10], we then carry out the steps that establish the connection between the Kubo formula and the Landauer-Büttiker formula.

2. Cohomology of electrical transport

We begin by reviewing some fundamental aspects of electrical transport theory in the mathematical context of a smooth d-dimensional manifold X. In the most general setting of that theory X is neither compact, nor need it be orientable.

Recall that on a differentiable manifold X one has the differential forms of degree k, namely $\Omega^k(X)$; the closed k-forms, $Z^k(X)$; and the exact k-forms, $B^k(X)$. The de Rham cohomology groups of X are the quotients $H^\bullet(X) = Z^\bullet(X)/B^\bullet(X)$.

In the most general setting, where X is not assumed to be orientable, one also needs the notion of twisted cohomology, which is summarized as follows. One defines the orientation bundle $L \to X$ as the real line bundle whose transition functions are given by the sign of the Jacobian. L is a *flat* vector bundle, meaning that the transition functions are locally constant. Twisted differential forms of degree k with values in a general flat vector bundle F then are sections of the tensor product bundle $\wedge^k(T^*X) \otimes F$. The vector space of twisted k-forms is denoted by $\Omega^k(X; F)$. The calculus of differential forms has a straightforward generalization to the twisted case. The exterior derivative d is well-defined with $\mathrm{d}^2 = 0$ since the transition functions of the twisting bundle are locally constant. Furthermore, e.g., there exists a canonical notion of pullback of vector bundle, and using it to pull back the sections of $\wedge^q(T^*M) \otimes F$ one defines $i^* : \Omega^q(M; F) \to \Omega^q(\partial M; F)$.

Closed and exact twisted k-forms are denoted by $Z^k(X; F)$ resp. $B^k(X; F)$. The cohomology groups of the twisted de Rham complex are

$$H^\bullet(X; F) = Z^\bullet(X; F)/B^\bullet(X; F) \ .$$

The significance of $F = L$ stems from the fact that integration of forms twisted by L can be defined even when the domain of integration fails to be orientable.

Compact support is indicated by a subscript 'c', e.g., $\Omega_c^k(X)$. The cohomology for compactly supported differential forms differs from the usual de Rham cohomology, but is related to it by the so-called intersection form, which is the operation of taking the wedge product and integrating:

$$H_c^q(X) \times H^{d-q}(X; L) \longrightarrow \mathbb{R} \ , \quad ([\xi], [\eta]) \mapsto \int_X \xi \wedge \eta \ .$$

Poincaré duality in this context, and under the weak condition of existence of a finite good cover for X, says that the intersection form is non-degenerate [3]. As a result one has isomorphisms

$$H_c^q(X) \cong H^{d-q}(X; L)^* \ .$$

We will presently use this isomorphism in the case of $q = 1$, viewing electrical voltages as linear functions on electrical currents.

2.1. **Charge and current density.** Finding the total amount of electric charge in a domain $U \subset X$ is a counting exercise that does not require U to be oriented or even orientable. Accordingly, in the continuum approximation one models [7, 4] the electric charge density ρ on X as a twisted d-form, $\rho \in \Omega^d(X; L)$. The electric charge $Q(U)$ in $U \subset X$ is computed from ρ by integration: $Q(U) = \int_U \rho$.

The electric current density, commonly denoted by j in physics, is the quantity that encodes the information about the flow of the electric charges. The proper mathematical model for it is a twisted $(d-1)$-form, $j \in \Omega^{d-1}(X;L)$. By integrating j over a $(d-1)$-dimensional submanifold S in X, one obtains the electric current through S:

$$I(S) := \int_S j\,.$$

$I(S)$ comes with a sign which depends on the choice of outer orientation of S (by which we mean a choice of direction of passing through the hypersurface S).

If S is a boundary, say $S = \partial U$, the law of conservation of electric charge says that $I(S) = -\frac{d}{dt}Q(U)$. The differential version of this law is $\mathrm{d}j = -\dot{\rho}$. Here and elsewhere the dot over a time-dependent quantity means the time derivative.

In a stationary situation where $\dot{\rho} = 0$, the electric current density $j \in \Omega^{d-1}(X, L)$ is closed: $\mathrm{d}j = 0$. If we are not interested in the fine details of j but want only its period integrals, i.e., integrals over closed hypersurfaces, then there is no loss in sending j to its twisted de Rham cohomology class, $[j] \in H^{d-1}(X;L)$. The cohomology class $I := [j]$ is called the (total) *current* for j.

2.2. **Current vector field.** From now on we assume that X carries a Riemannian structure. The Riemannian metric induces canonical scalar products, $\langle\cdot,\cdot\rangle$, on all tensor bundles as well as a volume density dvol_X. Moreover, the Hodge star operator, which is characterized by the identity

$$\omega_1 \wedge *\omega_2 = \langle\omega_1,\omega_2\rangle\,\mathrm{dvol}_X\,, \quad \omega_j \in \Omega^k(X;L) \text{ or } \omega_j \in \Omega^k(X), \tag{2.1}$$

gives isomorphisms

$$\Omega^k(X) \leftrightarrow \Omega^{d-k}(X;L)\,. \tag{2.2}$$

Furthermore, the metric induces natural isomorphisms between covariant and contravariant tensor fields. Explicitly, for a vector field $v \in \Gamma^\infty(TX)$ the corresponding one-form $v^\flat$ is characterized by $v^\flat(w) := \langle v, w\rangle$, $w \in \Gamma^\infty(TX)$. Composing $\flat$ with the $*$-operator we obtain an identification between vector fields and twisted $(d-1)$-forms. This will be used repeatedly in this paper, so we here record it.

Lemma 2.1. *On a Riemannian manifold X with volume density dvol_X the map from $\Gamma^\infty(TX)$ to $\Omega^{d-1}(X;L)$ given by $v \mapsto *v^\flat = \iota(v)\,\mathrm{dvol}_X$ is an isomorphism.*

Thus one may think of the electric current density j in terms of the vector field v which yields j upon contraction with dvol_X:

$$\iota(v)\,\mathrm{dvol}_X = j\,.$$

v is called the vector field of the electric current, or current vector field for short.

The divergence of a vector field v is defined via the Lie derivative $\mathscr{L}_v$ by

$$\mathscr{L}_v\,\mathrm{dvol}_X = \mathrm{div}(v)\,\mathrm{dvol}_X\,,$$

and by Cartan's formula, $\mathscr{L}_v = \mathrm{d}\,\iota(v) + \iota(v)\,\mathrm{d}$, taking the exterior derivative of $j = \iota(v)\,\mathrm{dvol}_X$ corresponds to taking the divergence of v:

$$\mathrm{d}j = \mathrm{div}(v)\,\mathrm{dvol}_X\,. \tag{2.3}$$

By the integral of the vector field v over a $(d-1)$-dimensional submanifold S we mean $\int_S v := \int_S \iota(v)\,\mathrm{dvol}_X$.

2.3. **Voltage.** The electric field strength is a 1-form, E, while the magnetic field strength is a 2-form, B. As part of Maxwell's theory the field strengths obey Faraday's law of induction: $\mathrm{d}E = -\dot{B}$. Thus E is closed if $\dot{B} = 0$. Let us then consider sending E to its cohomology class, $E \mapsto [E]$. In a strictly stationary situation, it is a postulate of physics that the electric field has an electric potential: $E = \mathrm{d}\Phi$, so the de Rham cohomology class $[E]$ is always trivial in that case.

However, there exist two reasons why in the physics problem at hand $[E]$ may still become nontrivial. Firstly, it may happen that $\dot{B} = 0$ inside the mesosopic conductor filling the region X, but $\dot{B} \neq 0$ somewhere outside. In that case E restricted to X is closed, but E need not be exact. Secondly, and more importantly, we will make the assumption (which is always made in mesoscopic conductor physics) that E vanishes outside some bounded region of space. The proper notion to use for E then is not the (de Rham) cohomology but rather the (de Rham) cohomology with compact supports, $[E] \in H_c^1(X)$. In the latter sense $[E]$ may be nonzero even in a truly stationary situation. $V := [E]$ is called the (static) voltage in physics.

2.4. **Conductivity as a map in cohomology.** Suppose that the electric charges of a physical system without external forces are at rest (so that $j = 0$). On imposing a driving force by means of an external electric field, one expects the system to respond with an electric current flow. For a sufficiently weak electric field the relation between E and j is linear in general, and one then calls the linear operator $\hat{\sigma} : E \mapsto j$ the linear-response electrical conductivity. In the stationary limit of interest to us, one attaches to $\hat{\sigma}$ the adjective 'd.c.' (standing for 'directed current' as opposed to 'alternating current', or 'a.c.').

Definition 2.2. The *d.c. linear-response electrical conductivity* is a linear mapping $\hat{\sigma} : \Omega_c^1(X) \to \Omega^{d-1}(X; L)$, $E \mapsto j = \hat{\sigma}(E)$ (depending, in general, on physical parameters such as gate voltages, magnetic fields, etc.) with the following properties.

- $\hat{\sigma}$ takes rotationless electric fields to divergenceless electric current densities, i.e., restricts to a linear mapping

$$\hat{\sigma} : Z_c^1(X) \longrightarrow Z^{d-1}(X; L) . \tag{2.4}$$

- The linear operator $\hat{\sigma}$ possesses a smooth integral kernel. Using the one-to-one correspondence between vector fields and twisted $(d-1)$-forms by $v \leftrightarrow \iota(v)\,\mathrm{dvol}_X$, one may view this kernel as a bi-vector field and express $j = \hat{\sigma}(E)$ in components with respect to some basis as

$$\hat{\sigma}(E)^i(x) = \int_X \sigma^{ii'}(x, x') E_{i'}(x')\,\mathrm{dvol}_X(x') . \tag{2.5}$$

- The components of the bi-vector field of $\hat{\sigma}$ obey the Onsager relation

$$\sigma^{ii'}(x, x'; B) = \sigma^{i'i}(x', x\,; -B) . \tag{2.6}$$

  In words: changing the sign of the magnetic field strength B (and, more generally, changing the sign of all physical parameters that are odd w.r.t. time inversion) sends the bi-vector field of $\hat{\sigma}$ to its transpose.

Remark 2.3. There exists a consensus among physicists [1] that any reasonable theory of d.c. linear response has to satisfy the properties asserted in Def. 2.2.

For the following statement and proof it will be helpful to have another notation. If $\mathbf{x} = (x; v_1, \ldots, v_{d-1})$ with $x \in X$ and $v_i \in T_x X$, let $j(\mathbf{x}) := j_x(v_1, \ldots, v_{d-1})$, and going back to the primary definition of the integral kernel of $\hat{\sigma}$ as a twisted bi-differential form of degree $d - 1$, introduce the short-hand notation

$$\sigma(\mathbf{x}\,, \mathbf{x}') := \sigma_{x,x'}(v_1, \ldots, v_{d-1}; v_1', \ldots, v_{d-1}') .$$

(2.5) then takes the invariant form

$$j(\mathbf{x}) = \hat{\sigma}(E)(\mathbf{x}) = \int_X \sigma(\mathbf{x}\,, \cdot) \wedge E .$$

The situation at hand involves two cochain complexes: the twisted de Rham complex $(\Omega^*(X; L), \mathrm{d})$, and the cochain complex of compactly supported forms, $(\Omega_c^*(X), \mathrm{d})$. In algebraic topology, a linear mapping between (co)chain complexes is called a chain map if it commutes with the differential operator d. Our electrical conductivity is not a chain map, but does share the following property.

Proposition 2.4. *Under the postulates* (2.4–2.6) *above, the d.c. linear-response electrical conductivity descends to a map in cohomology,* $H_c^1(X) \to H^{d-1}(X; L)$.

Proof. Given that $\hat{\sigma}$ takes closed forms to closed forms by postulate (2.4), there is a well-defined induced map in cohomology if $\hat{\sigma}(B_c^1(X)) \subset B^{d-1}(X; L)$. Thus, the statement to be proved is that if $E = \mathrm{d}\Phi$ with compactly supported Φ, then the twisted $(d-1)$-form $j = \hat{\sigma}(E)$ is exact.

For notational clarity, we denote in this proof by d_1, d_2 the exterior derivatives with respect to the first resp. second argument of $\hat{\sigma}$. Our proof starts by integrating $\mathrm{d}_2\Phi \wedge \sigma(\mathbf{x}, \cdot) = \mathrm{d}_2 (\Phi\, \sigma(\mathbf{x}, \cdot)) - \Phi\, \mathrm{d}_2\sigma(\mathbf{x}, \cdot)$ over X. By Stokes' theorem for the compactly supported form $\mathrm{d}_2 (\Phi\sigma(\mathbf{x}, \cdot))$ this leads to

$$\hat{\sigma}(\mathrm{d}\Phi)(\mathbf{x}) = \pm \int_X \Phi\, \mathrm{d}_2\sigma(\mathbf{x}, \cdot) \; .$$

Since $j = \hat{\sigma}(\mathrm{d}\Phi)$ is closed for any function Φ by postulate (2.4), it follows that

$$\mathrm{d}_1\mathrm{d}_2\sigma(\cdot', \cdot) = 0 \; , \tag{2.7}$$

i.e., the bi-differential form σ becomes zero when an exterior derivative is applied to each of its two sets of variable arguments.

Now integrate the closed form $\mathrm{d}_2\sigma(\cdot, \mathbf{x}')$ (with variable first and fixed second argument) against any compactly supported closed test form $\eta \in Z_c^1(X)$. Using the Onsager relation (2.6) and moving the primed exterior derivative in front of the integral over unprimed variables, one gets

$$\int_X \mathrm{d}_2\sigma(\cdot\, , \mathbf{x}'; B) \wedge \eta = \mathrm{d}_1 \int_X \sigma(\mathbf{x}', \cdot\, ; -B) \wedge \eta = 0 \; .$$

The right-hand side is zero, again by virtue of (2.4). It follows that $\hat{\sigma}(\mathrm{d}\Phi)$ vanishes on integration against any closed form $\eta \in Z_c^1(X)$:

$$\int_X \hat{\sigma}(\mathrm{d}\Phi)\Big|_B \wedge \eta = \pm \int_X' \Phi(\cdot') \int_X \mathrm{d}_2\sigma(\cdot, \cdot'; B) \wedge \eta = 0 \; .$$

By Poincaré duality, $H_c^1(X) \cong H^{d-1}(X; L)^*$, this implies that $\hat{\sigma}(\mathrm{d}\Phi)$ is exact. $\square$

2.5. **Conductance.** We have shown that the d.c. linear-response electrical conductivity $\hat{\sigma} : Z_c^1(X) \to Z^{d-1}(X; L)$ descends to a mapping in cohomology. This map, taking voltages $V = [E] \in H_c^1(X)$ to currents $I = [j] \in H^{d-1}(X; L)$, has a special name in physics.

Definition 2.5. The induced map,

$$G : \; H_c^1(X) \longrightarrow H^{d-1}(X; L) \; ,$$

is called the d.c. linear-response electrical *conductance*.

Remark 2.6. By Poincaré duality, one can reformulate the conductance as

$$G : \; H_c^1(X) \cong H^{d-1}(X; L)^* \xrightarrow{\;g\;} H^{d-1}(X; L) \; ,$$

where g, being a map between a vector space and its dual, has a canonical adjoint (or transpose), g^*. The Onsager relation (2.6) restated at the cohomological level then says that

$$g(B)^* = g(-B) \; .$$

Thus in the absence of magnetic fields (and other parameters that break time-reversal symmetry) the conductance g is symmetric.

While Def. 2.5 makes no reference to the physical system being ‘open’ or ‘closed’, our interest in the present paper will be in the electrical transport of a certain class of open systems. These are constructed by taking a compact manifold M with boundary $\partial M = Y$ and gluing the product $\mathbb{R}_+ \times Y$ to M along the common boundary to form

$$X := M \cup_{\partial M} (\mathbb{R}_+ \times Y) \,. \tag{2.8}$$

Y consists of several connected components Y_α ($\alpha = 1, \ldots, N$) in general. We say that the noncompact manifold X has cylindrical ends $\mathbb{R}_+ \times Y_\alpha$.

On such a manifold X we distinguish between two kinds of electrical current $I \in H^{d-1}(X; L)$: currents flowing between the cylindrical ends of X are called transport currents, while those circulating around non-contractible loops (if any) of M are called inner currents. Motivated by the circumstance that the inner currents might not be measured experimentally, we wish to remove these currents to arrive at a mathematical framework that sees only the transport currents.

The good notion to use for that purpose is that of the *relative* de Rham cohomology determined by the inclusion $i : \partial M \to M$. There are three cochain complexes which compute the relative de Rham cohomology, and for the convenience of the reader we are going to summarize the facts in some detail. In order to treat the twisted and the untwisted case simultaneously, we consider an auxiliary flat vector bundle F and de Rham theory with coefficients in F. In the untwisted case $F = \mathbb{R}$ is the trivial line bundle, while in the non-oriented case we may choose F to be the orientation line bundle L. Let

$$\Omega^q_0(M, \partial M; F) := \big\{\omega \in \Omega^q(M; F) \;\big|\; i^*\omega = 0\big\}$$

be the kernel of the pullback i^*. Then we have an exact sequence

$$0 \longrightarrow \Omega^*_0(M, \partial M; F) \xrightarrow{\alpha} \Omega^*(M; F) \xrightarrow{i^*} \Omega^*(\partial M; F) \longrightarrow 0, \tag{2.9}$$

where α is the inclusion map. Furthermore, the *mapping cone* of i^* is the cochain complex $\Omega^*_{\mathrm{rel}}(M, \partial M; F) = \oplus_{q\geq 0}\, \Omega^q_{\mathrm{rel}}(M, \partial M; F)$,

$$\Omega^q_{\mathrm{rel}}(M, \partial M; F) = \Omega^q(M; F) \oplus \Omega^{q-1}(\partial M; F) \,, \tag{2.10}$$

with differential

$$\mathrm{d} :\, (\omega, \theta) \mapsto (\mathrm{d}\omega, i^*\omega - \mathrm{d}\theta) \,, \quad \omega \in \Omega^q(M) \,, \quad \theta \in \Omega^{q-1}(\partial M) \,.$$

Note that if (ω, θ) represents a cohomology class in $H^q_{\mathrm{rel}}(M, \partial M; F)$, then ω is a closed q-form on M which restricts to an exact form $i^*\omega = \mathrm{d}\theta$ on ∂M.

With the natural chain maps

$$\begin{aligned} &\beta :\, \Omega^{q-1}(\partial M; F) \longrightarrow \Omega^q_{\mathrm{rel}}(M, \partial M; F), \quad \theta \mapsto (0, (-1)^{q-1}\theta), \\ &\gamma :\, \Omega^q_{\mathrm{rel}}(M, \partial M; F) \longrightarrow \Omega^q(M; F), \quad (\omega, \theta) \mapsto \omega \,, \end{aligned}$$

we obtain a second exact sequence of cochain complexes involving $\Omega^*(M; F)$ and $\Omega^*(\partial M; F)$:

$$0 \longrightarrow \Omega^{*-1}(\partial M; F) \xrightarrow{\beta} \Omega^*_{\mathrm{rel}}(M, \partial M; F) \xrightarrow{\gamma} \Omega^*(M; F) \longrightarrow 0 \,. \tag{2.11}$$

There is a natural inclusion of cochain complexes

$$\varepsilon :\, \Omega^*_0(M, \partial M; F) \longrightarrow \Omega^*_{\mathrm{rel}}(M, \partial M; F), \quad \omega \mapsto (\omega, 0) \,.$$

It is straightforward to check that the long exact cohomology sequences of (2.9) and (2.11) are connected by the following (sign) commutative diagram

$$\begin{array}{ccccccc} \cdots H_0^q(M,\partial M) & \xrightarrow{\alpha_*} & H^q(M) & \xrightarrow{i^*} & H^q(\partial M) & \xrightarrow{\delta} & H_0^{q+1}(M,\partial M)\cdots \\ \downarrow \varepsilon & & \downarrow \mathrm{id} & & \downarrow \mathrm{id} & & \downarrow \varepsilon \\ \cdots H_{\mathrm{rel}}^q(M,\partial M) & \xrightarrow{\gamma_*} & H^q(M) & \xrightarrow{\delta} & H^q(\partial M) & \xrightarrow{\beta_*} & H_{\mathrm{rel}}^{q+1}(M,\partial M)\cdots \end{array} \tag{2.12}$$

(where the symbol F is omitted for brevity) and therefore, by the Five Lemma, ε is a quasi-isomorphism of cochain complexes, i.e., ε_* is an isomorphism.

Hence the cochain complexes $\Omega_0^*(M,\partial M;F)$ and $\Omega_{\mathrm{rel}}^*(M,\partial M;F)$ both compute the *relative* de Rham cohomology with coefficients in F of the pair $(M,\partial M)$. In fact this relative cohomology is nothing but the cohomology with compact support of the open manifold $\overset{\circ}{M}:= M\setminus\partial M$:

Lemma 2.7. *The natural inclusions*

$$\Omega_c^*(\overset{\circ}{M};F) \xrightarrow{\varepsilon_1} \Omega_0^*(M,\partial M;F) \xrightarrow{\varepsilon_2} \Omega_{\mathrm{rel}}^*(M,\partial M;F)$$

induce maps $\varepsilon_{j,*}$ in cohomology which are isomorphisms $(j=1,2)$. The pairing

$$H_{\mathrm{rel}}^q(M,\partial M)\otimes H^{d-q}(M;L)\to\mathbb{R}\ , \quad [(\omega,\theta)]\otimes[\eta]\mapsto\int_M\omega\wedge\eta-\int_{\partial M}\theta\wedge i^*\eta\ ,$$

is well-defined and extends the intersection pairing $H_c^q(\overset{\circ}{M})\otimes H^{d-q}(M;L)\longrightarrow\mathbb{R}$ through $\varepsilon_2\circ\varepsilon_1$.

Proof. For ε_2 the claim follows from the (sign) commutative diagram (2.12). We will present, however, an ad hoc proof which works for ε_1 and ε_2 simultaneously. Let us first prove the following:

Claim. *Let $\omega\in\Omega^q(M;F)$ such that there is a $\theta\in\Omega^{q-1}(\partial M;F)$ with $i^*(\omega)=\mathrm{d}\theta$ and $\mathrm{d}(\omega|_U)=0$ for a collar neighborhood U of ∂M. Then there is a $\xi\in\Omega^{q-1}(M;F)$ with $i^*\xi=\theta$ and $\mathrm{d}(\xi|_V)=\omega$ in a maybe smaller collar neighborhood V of ∂M.*

To see this, we note that the collar neighborhood $U\simeq[0,1)\times\partial M$ is homotopically equivalent to ∂M and hence $i^*: H^q(U;F)\to H^q(\partial M;F)$ is an isomorphism. Therefore, since $i^*\omega$ is exact, there exists $\xi_1\in\Omega^{q-1}(U;F)$ with $\mathrm{d}\xi_1=\omega|_U$. Denoting by $\pi: U\to\partial M$ the natural projection, we put $\xi_2:=\xi_1+\pi^*\theta-\pi^*i^*\xi_1$. Then $\mathrm{d}\xi_2=\omega|_U$ and $i^*\xi_2=\theta$. Using a cut-off function we now find a smooth form $\xi\in\Omega^{q-1}(M;F)$ which agrees with ξ_2 in a suitable collar neighborhood V of ∂M.

Returning to the proof of the Lemma we now show that $(\varepsilon_2\circ\varepsilon_1)_*$ is injective:

Let $\omega\in\Omega_c^q(\overset{\circ}{M};F)$ with $\mathrm{d}\omega=0$ and assume that $(\omega,0)=\mathrm{d}(\eta,\theta)=(\mathrm{d}\eta,i^*\eta-\mathrm{d}\theta)$ for some $\eta\in\Omega^{q-1}(M;F)$, $\theta\in\Omega^{q-2}(\partial M;F)$. Since ω has compact support in the interior of $M\setminus\partial M$ we may apply the Claim to the form η and find a $\xi\in\Omega^{q-2}(M;F)$ with $i^*\xi=\theta$ and $\mathrm{d}\xi|_U=\eta|_U$ in a collar neighborhood of ∂M. The form $\eta-\mathrm{d}\xi$ then has compact support and $\mathrm{d}(\eta-\mathrm{d}\xi)=\omega$. Hence ω is exact in $\Omega_c^q(\overset{\circ}{M};F)$.

To prove surjectivity of $(\varepsilon_2\circ\varepsilon_1)_*$ let $(\omega,\theta)\in\Omega_{\mathrm{rel}}^q(M,\partial M;F)$ be closed, i.e., $\mathrm{d}\omega=0$, $i^*\omega=\mathrm{d}\theta$. We apply the Claim to ω and find $\xi\in\Omega^{q-1}(M;F)$ with $\mathrm{d}\xi=\omega$ in a collar neighborhood of ∂M and $i^*\xi=\theta$. Then $(\omega,\theta)-\mathrm{d}(\xi,0)=(\omega-\mathrm{d}\xi,0)=\varepsilon_2(\varepsilon_1(\omega))$, hence the cohomology class of (ω,θ) is represented by the image of the compactly supported form $\omega-\mathrm{d}\xi$.

Surjectivity of ε_1 is proved the same way. The statement about the intersection pairing follows immediately from Stokes' Theorem. ∎

The open manifold $\overset{\circ}{M}$ is diffeomorphic (but of course not isometric) to the manifold $X = M \cup_{\partial M} (\mathbb{R}_+ \times Y)$ obtained by attaching cylinders to the boundary. Therefore $H^q_c(X;F)$ is naturally isomorphic to $H^q_{\mathrm{rel}}(M,\partial M;F)$. Let us describe this isomorphism in more concrete terms:

Denote by π the projection map

$$\pi:\ \mathbb{R}_+ \times Y \longrightarrow Y\ , \quad (r,y) \mapsto y\ .$$

Integration over the fiber $\mathbb{R}_+$ of π yields a mapping of differential forms,

$$\pi_*:\ \Omega^q_c(\mathbb{R}_+ \times Y) \to \Omega^{q-1}(Y)\ .$$

Using it one gets a linear mapping

$$\Omega^q_c(X) \ni \omega \mapsto (\omega|_M\ , -\pi_*\omega|_{\mathbb{R}_+\times Y}) \in \Omega^q_{\mathrm{rel}}(M,\partial M)\ . \tag{2.13}$$

It is straightforward to check that the mapping (2.13) is a chain map. If a form ω has compact support in $\overset{\circ}{M}$ then the map (2.13) sends ω to $(\omega,0)$. Since $H^q_c(X;F)$ is isomorphic to $H^q_c(\overset{\circ}{M};F)$ every cohomology class in $H^q_c(X;F)$ may be represented in this way and we have proved

Lemma 2.8. *The mapping* (2.13) *induces an isomorphism of cohomology groups*

$$H^*_c(X) \longrightarrow H^*_{\mathrm{rel}}(M,\partial M)\ , \quad [\omega] \mapsto [(\omega|_M, -\pi_*\omega|_{\mathbb{R}_+\times Y})]\ ,$$

which sends the intersection form $H^q_c(X) \otimes H^{d-q}(X;L) \to \mathbb{R}$ to the pairing

$$H^q_{\mathrm{rel}}(M,\partial M) \otimes H^{d-q}(M;L) \to \mathbb{R}\ , \quad [(\varepsilon,\phi)] \otimes [\eta] \mapsto \int_M \varepsilon \wedge \eta - \int_{\partial M} \phi \wedge i^*\eta\ .$$

Note that, since M is a deformation retract of X, the cohomology $H^*(X;L)$ is canonically isomorphic to $H^*(M;L)$.

Of course the intersection pairing $H^q_{\mathrm{rel}}(M,\partial M) \otimes H^{d-q}(M;L) \to \mathbb{R}$ is still non-degenerate. This has the following consequence.

Corollary 2.9. *In the setting of $X = M \cup_{\partial M} (\mathbb{R}_+ \times Y)$, the electrical conductance $G:\ H^1_c(X) \to H^{d-1}(X;L)$ may be regarded as a map*

$$G:\ H^1_{\mathrm{rel}}(M,\partial M) \longrightarrow H^{d-1}(M;L) \cong H^1_{\mathrm{rel}}(M,\partial M)^*\ .$$

2.6. **Transport conductance.** Consider now some cohomology class

$$[(j\,,\theta)] \in H^{d-1}_{\mathrm{rel}}(M,\partial M;L)\ ,$$

which means that j is a closed twisted $(d-1)$-form on M which becomes exact upon restriction to the boundary ∂M. By Stokes theorem, the latter property implies that $\int_{Y_\alpha} j$ vanishes for each boundary component $Y_\alpha \subset Y = \partial M$. Thus a current $I \in H^{d-1}_{\mathrm{rel}}(M,\partial M;L)$ is what we call an inner current. When combined with the fact that $H^*(X;L)$ is isomorphic to $H^*(M;L)$, this observation will allow us to eliminate the interior currents by taking a quotient of $H^{d-1}(M;L)$ by $H^{d-1}_{\mathrm{rel}}(M,\partial M;L)$.

What is the corresponding reduction on the voltage side? To answer that, we consider the long exact cohomology sequence of the short exact sequence (2.11):

$$\ldots \longrightarrow H^{q-1}(M) \xrightarrow{i^*} H^{q-1}(\partial M) \xrightarrow{\beta_*} H^q_{\mathrm{rel}}(M,\partial M) \xrightarrow{\gamma_*} H^q(M) \longrightarrow \ldots\ . \tag{2.14}$$

Then we set $q = 1$ and consider some element

$$\phi = (\phi_1,\phi_2,\ldots,\phi_N) \in H^0(\partial M)\ ,$$

where each ϕ_α is a number (in physics language: an electric potential value), viewed as a constant function on the corresponding boundary component $Y_\alpha \subset Y = \partial M$. The map β_* sends ϕ to

$$[(0,\phi)] \in \beta_* H^0(\partial M) \subset H^1_{\mathrm{rel}}(M,\partial M)\ .$$

To interpret $[(0,\phi)]$ note that if $\Phi: M \to \mathbb{R}$ satisfies the condition $i^*\Phi = \phi$, then

$$[(0,\phi)] = [(0,\phi)] - [(\mathrm{d}\Phi, i^*\Phi)] = [(-\mathrm{d}\Phi, 0)] .$$

Thus the cohomology class $[(0,\phi)] \in \beta_* H^0(\partial M)$ corresponds to the class of exact electric field strengths $E = -\mathrm{d}\Phi$ on M which assume the given boundary values $i^*\Phi = \phi$ on ∂M. We call $[(0,\phi)] = [(-\mathrm{d}\Phi, 0)]$ an 'outer' voltage.

Definition 2.10. Given the full conductance $G: H^1_{\mathrm{rel}}(M, \partial M) \to H^{d-1}(M; L)$, one defines the *transport* conductance as the restricted map

$$G_{\mathrm{tr}}: \beta_* H^0(\partial M) \to H^{d-1}(M; L)/\gamma_* H^{d-1}_{\mathrm{rel}}(M, \partial M; L) .$$

Thus in the transport setting at hand, one prepares the electric field E in such a way that only an outer voltage $V \in \beta_* H^0(\partial M)$ is present (and no inner or ring voltage), and one chooses not to observe the inner current $I \in H^{d-1}_{\mathrm{rel}}(M, \partial M; L)$.

The following statement prepares our final formulation of transport conductance.

Lemma 2.11. *The intersection form* $H^q_{\mathrm{rel}}(M, \partial M) \otimes H^{d-q}(M; L) \to \mathbb{R}$ *restricts to a non-degenerate pairing*

$$\beta_* H^{q-1}(\partial M) \otimes H^{d-q}(M; L)/\gamma_* H^{d-q}_{\mathrm{rel}}(M, \partial M; L) \longrightarrow \mathbb{R} .$$

Proof. Denote the intersection pairing by $\langle \cdot, \cdot \rangle$ and note that for $[\theta] \in H^{q-1}(\partial M)$, $[\omega] \in H^{d-q}(M; L)$ we have in view of Lemma 2.7

$$\begin{aligned} \langle \beta_*[\theta], [\omega] \rangle &= \langle [(0, (-1)^{q-1}\theta)], [\omega] \rangle \\ &= (-1)^q \int_{\partial M} \theta \wedge i^*\omega = (-1)^q \langle [\theta], i^*[\omega] \rangle, \end{aligned} \tag{2.15}$$

where the pairing on the right-hand side is the intersection pairing on the boundary ∂M. If $[\omega] = \gamma_*[(\omega, \xi)]$ with $[(\omega, \xi)] \in H^{d-q}_{\mathrm{rel}}(M, \partial M; L)$ then $i^*[\omega] = [\mathrm{d}\xi] = 0$ and hence by (2.15)

$$\langle \beta_*[\theta], [\omega] \rangle = \pm \langle [\theta], i^*[\omega] \rangle = 0 .$$

Therefore (2.15) induces a well-defined bilinear pairing

$$\beta_* H^{q-1}(\partial M) \otimes H^{d-q}(M; L)/\gamma_* H^{d-q}_{\mathrm{rel}}(M, \partial M; L) \to \mathbb{R} .$$

Furthermore, if $\langle \beta_*[\theta], [\omega] \rangle = 0$ for all $[\omega] \in H^{d-q}(M; L)/\gamma_* H^{d-q}_{\mathrm{rel}}(M, \partial M; L)$ then the non-degeneracy of the relative intersection pairing implies $\beta_*[\theta] = 0$.

Conversely, if $0 = \langle \beta_*[\theta], [\omega] \rangle = \pm \langle [\theta], i^*[\omega] \rangle$ for all $[\theta] \in H^{q-1}(\partial M)$ then the non-degeneracy of the intersection pairing on ∂M implies $i^*[\omega] = 0$ and hence $[\omega] \in \gamma_* H^{d-q}_{\mathrm{rel}}(M, \partial M; L)$. □

Using physics terminology one could say that, w.r.t. the pairing given by the electrical power $\int E \wedge j$, outer voltages annihilate inner currents and vice versa.

By Lemma 2.11 the quotient space $H^{d-1}(M; L)/\gamma_* H^{d-1}_{\mathrm{rel}}(M, \partial M; L)$ is isomorphic to the dual vector space of $\beta_* H^0(\partial M)$. Since $\beta_* H^0(\partial M) \cong H^0(\partial M)/i^* H^0(M)$ by exactness of the sequence (2.14), this leads us to the final formulation of the transport conductance as a mapping

$$G_{\mathrm{tr}}: \mathscr{V} \longrightarrow \mathscr{V}^*, \quad \mathscr{V} = H^0(\partial M)/i^* H^0(M) . \tag{2.16}$$

Notice that since M is connected and ∂M has N connected components, one has $\mathscr{V} = H^0(\partial M)/i^* H^0(M) \cong \mathbb{R}^{N-1}$. We may think of $\mathscr{V}$ as the vector space of outer voltages, i.e., the set of potential differences between pairs of cylindrical ends. On that space, the transport conductance $G_{\mathrm{tr}}: \mathscr{V} \to \mathscr{V}^*$ determines a bilinear form

$$P: \mathscr{V} \times \mathscr{V} \to \mathbb{R}, \quad (V, V') \mapsto G_{\mathrm{tr}}(V)(V') ,$$

expressing the electrical power in terms of the outer voltages alone.

2.7. **Conductance as a double flux integral.** For the purpose of further analysis we need a convenient prescription for computing $G_{\rm tr}$ from a given conductivity bi-vector field σ. It should be evident now how to do this. Choose a basis of homology generators $\{Y_1, \ldots, Y_N\}$ of $H_{d-1}(\partial M)$, i.e., a set of N cross sections Y_α, one for each cylindrical lead. Let the orientation of each Y_α be given by the normal vector pointing outwards. Viewing the conductivity as a twisted double differential form σ of degree $d-1$ by the isomorphism $\Gamma^\infty(TX) \cong \Omega^{d-1}(X; L)$, compute the double current flux integrals

$$(G_{\rm tr})_{\alpha\beta} := -\int_{x_\alpha \in Y_\alpha} \int_{x_\beta \in Y_\beta} \sigma(x_\alpha, x_\beta) \; . \tag{2.17}$$

The electrical power then is

$$P(V) = G_{\rm tr}(V)(V) = \sum_{\alpha,\beta=1}^{N} (G_{\rm tr})_{\alpha\beta} V_\alpha V_\beta \; .$$

This descends to a quadratic form on the quotient $\mathscr{V} = H^0(\partial M)/i^* H^0(M)$ because $\sum_\alpha (G_{\rm tr})_{\alpha\beta} = \sum_\beta (G_{\rm tr})_{\alpha\beta} = 0$.

3. Conductivity from quantum mechanics

So far, our considerations have required no more than the setting of classical particles and fields. Now, extending our framework to the quantum mechanics of charged particles (in the first-quantized theory), we consider a Hamiltonian operator D defined on the sections of a Hermitian vector bundle E over X. We review how such an operator is associated with a divergenceless current vector field v_D by the principle of minimal substitution. While such a vector field can always be found, one needs a covariant derivative ∇ for E in order for v_D to be defined uniquely. We distill from this construction a notion of *current operator*, which we use to associate with a pair of integral kernels K_1 and K_2 a certain bi-vector field $\Sigma(K_1, K_2)$. The significance of Σ is that on inserting the resolvent kernel of D into it, we obtain the Kubo expression for the electrical conductivity.

3.1. **Quantum-theoretic framework.** We now assume that we are given some extension of the classical framework of Sect. 2 to a framework for charged quantum particles. Let us briefly review what are the key features involved.

Building on the basic setting of a Riemannian manifold X, the axioms of quantum mechanics require that there be a Hermitian vector bundle $\pi : E \to X$, where for each $x \in X$ the fibre $E_x \cong \mathbb{C}^r$ carries a Hermitian scalar product $u, v \mapsto h_x(u, v)$. (By the standard conventions of quantum physics, h_x is complex linear in the second argument and complex anti-linear in the first argument.) The Hermitian vector bundle E is supposed to be equipped with a compatible covariant derivative ∇.

In this geometric setting, sections of E play the role of what physicists call the quantum mechanical 'wave function'. We denote the space of smooth sections of $\pi : E \to X$ by $\Gamma^\infty(E)$, and indicate compact support by a subscript c as before. The scalar product of two sections $\varphi, \psi \in \Gamma_c^\infty(E)$ is defined to be the integral

$$(\varphi, \psi) := \int_X h(\varphi, \psi) \, \mathrm{dvol}_X \; . \tag{3.1}$$

The quantum-theoretic Hilbert space is the L^2-space of square-integrable sections, $L^2(X, E)$. If a section $\psi \in L^2(X, E)$ is normalized by $\int_X h(\psi, \psi) \, \mathrm{dvol}_X = 1$, then the probability density for particles in the quantum state ψ is $h(\psi, \psi) \, \mathrm{dvol}_X$.

Let now the quantum particles with wave functions $\psi \in L^2(X, E)$ be coupled to the U(1) gauge field of Maxwell's theory. Since our aim is to handle a static situation, there is no need here to set up the full-fledged apparatus of Maxwell electrodynamics; rather, for our purpose of studying stationary electric current densities it suffices to have the mathematical structure of a U(1)-principal bundle P over X. Indeed, by the postulates of Maxwell's theory the electric current density is paired with the magnetic gauge potential, which in turn is given by a connection 1-form $\mathrm{i}A$ on P. We again follow the conventions of physics: A takes values in $\mathbb{R}$ so that $\mathrm{i}A$ takes values in $\mathfrak{u}(1)$. Changing the magnetic field amounts to replacing A by $A + A'$ where A' is a real-valued 1-form on X. By the principle of *minimal substitution*, the corresponding change of covariant derivative is $\nabla \to \nabla + \mathrm{i}A'$.

By $\mathrm{Diff}(E)$ we denote the space of differential operators on $\Gamma^\infty(E)$. An operator $D \in \mathrm{Diff}(E)$ always has a unique formal adjoint $D^\dagger \in \mathrm{Diff}(E)$, which is determined by the equation

$$(\varphi\,, D\psi) = (D^\dagger\varphi\,, \psi) \tag{3.2}$$

for all L^2-sections in the domain of D resp. $D^\dagger$.

In the following we consider only those differential operators D which are given to us by a unique expression in terms of the covariant derivative ∇ and of local tensor fields that are invariant under $A \to A+A'$. For such operators, changing the magnetic field $\nabla \to \nabla + \mathrm{i}A'$ causes $D = D_\nabla$ to change as $D_\nabla \to D_{\nabla+\mathrm{i}A'}$. (When the dependence of D on ∇ matters, we write D_∇ instead of just D.)

Example 3.1. The prime example to be pursued in this paper is that of a generalized Dirac operator $D = c(\mathrm{d}x^i)\nabla_{\partial/\partial x^i}$ where $c : T^*X \to \mathrm{End}(E)$, the Clifford bundle map, is odd w.r.t. a $\mathbb{Z}_2$-grading $E = E^+ \oplus E^-$ and obeys the relations

$$c(e^i)c(e^j) + c(e^j)c(e^i) = -2\delta^{ij}$$

for orthonormal frames $\{e^i\}$ of T^*X. Variation of the magnetic gauge potential $A \to A + A'$ in this case results in $D \to D + \mathrm{i}c(A')$.

Let there now be a distinguished differential operator $D = D^\dagger \in \mathrm{Diff}(E)$, called the *Hamiltonian*, which determines the evolution with time t of the quantum system by the equation

$$(D - \mathrm{i}\partial_t)\psi = 0\,. \tag{3.3}$$

Assuming that each quantum particle carries one unit of electric charge, the electric charge density ρ can be identified with the probability density: $\rho = h(\psi, \psi)\,\mathrm{dvol}_X$. Then from (3.3) the time derivative of ρ is

$$\dot\rho = \big(- \mathrm{i}h(\psi, D\psi) + \mathrm{i}h(D\psi, \psi)\big)\,\mathrm{dvol}_X\ . \tag{3.4}$$

Next we associate with $\psi \in \Gamma_c^\infty(E)$ (at some fixed time t) an energy $H_\psi \in \mathbb{R}$ by

$$H_\psi := (\psi, D\psi) = \int_X h(\psi, D\psi)\,\mathrm{dvol}_X\ .$$

By the principles of quantum theory, the electric current density in the quantum state with wave function ψ is given by the first variation of H_ψ with respect to the magnetic potential. Thus, viewing the linear functional

$$\Omega_c^1(X) \longrightarrow \mathbb{R}\ , \quad A' \mapsto \frac{d}{ds}(\psi, D_{\nabla+\mathrm{i}sA'}\psi)\Big|_{s=0}$$

as arising from integration against a twisted differential form $j \in \Omega^{d-1}(X; L)$, one defines the electric current density j by the equation

$$\int_X A' \wedge j := \frac{d}{ds}(\psi, D_{\nabla+\mathrm{i}sA'}\psi)\Big|_{s=0}\ . \tag{3.5}$$

Let us verify that this j satisfies the continuity equation $\mathrm{d}j = -\dot\rho$. For that purpose, one puts $A' = \mathrm{d}f$ with arbitrary $f \in \Omega_c^0(X)$ and observes that the change of covariant derivative $\nabla \to \nabla + \mathrm{i}\mathrm{d}f$ can be seen as a conjugation, $\nabla \to \mathrm{e}^{-\mathrm{i}sf}\nabla \circ \mathrm{e}^{\mathrm{i}sf}$. One then has $D_{\nabla+\mathrm{i}s\mathrm{d}f} = \mathrm{e}^{-\mathrm{i}sf} D_\nabla \circ \mathrm{e}^{\mathrm{i}sf}$, and partial integration gives

$$-\int_X f\mathrm{d}j = \int_X \mathrm{d}f \wedge j = \frac{d}{ds}(\psi, \mathrm{e}^{-\mathrm{i}sf} D\, \mathrm{e}^{\mathrm{i}sf}\psi)\Big|_{s=0} = (\psi, [D, \mathrm{i}f]\psi) \ .$$

From this and the definition of the scalar product in (3.1) it follows that

$$\mathrm{d}j = \mathrm{i}\big(h(\psi, D\psi) - h(D\psi, \psi)\big)\, \mathrm{dvol}_X \ . \tag{3.6}$$

By comparing with (3.4) one sees that the right-hand side indeed is equal to $-\dot{\rho}$.

Example 3.2. Consider the Laplacian of the bundle E, i.e., the operator expressed in a local orthonormal frame $\{e_i\}$ of TX as $D = \delta^{ij}\nabla^\dagger_{e_i}\nabla_{e_j}$. In this case one finds that

$$j = \star\big(\mathrm{i}h(\nabla\psi, \psi) - \mathrm{i}h(\psi, \nabla\psi)\big) \ ,$$

with $\star : \Omega^1(X) \to \Omega^{d-1}(X; L)$ being the Hodge star operator of X.

3.2. **Current operator.** We shall need a slight generalization of the previous construction of the electric current density. So, fixing an operator $D \in \mathrm{Diff}(E)$ (and dropping the condition $D = D^\dagger$ for now), let there be in addition to ψ a second section $\varphi \in \Gamma^\infty_c(E)$, and consider the complex number

$$(\varphi\,, D\psi) = \int_X h(\varphi\,, D\psi)\, \mathrm{dvol}_X \ .$$

By varying this with respect to the magnetic gauge potential as before, we associate with the pair of sections $\varphi\,, \psi$ a complex-valued twisted $(d-1)$-form $j(\psi, \varphi)$:

$$\int_X A' \wedge j(\psi, \varphi) := \frac{d}{ds}(\varphi\,, D_{\nabla+\mathrm{i}sA'}\psi)\Big|_{s=0} \ . \tag{3.7}$$

The same computation that led to (3.6) now gives

$$\mathrm{d}j(\psi, \varphi) = \mathrm{i}\big(h(\varphi\,, D\psi) - h(D^\dagger\varphi\,, \psi)\big)\, \mathrm{dvol}_X \ . \tag{3.8}$$

Notice that since D is a differential operator, if A' is compactly supported then the right-hand side of (3.7) makes sense (after taking d/ds inside the scalar product) even without the assumption of compact support for ψ and φ.

Let us summarize this situation in terms of the current vector field of j.

Definition 3.3. For a pair of sections $\varphi\,, \psi \in \Gamma^\infty(E)$ let $j(\psi, \varphi) \in \Omega^{d-1}(X; L \otimes \mathbb{C})$ be the differential form determined by (3.7). We then define the *current operator* to be the mapping

$$\Gamma^\infty(E) \otimes_{\mathbb{R}} \Gamma^\infty(E) \to \Gamma^\infty(TX \otimes \mathbb{C}) \ , \quad \psi \otimes \varphi \mapsto v(\psi, \varphi) \ ,$$

where $v(\psi, \varphi)$ is the vector field that results from $j(\psi, \varphi)$ by applying the inverse of the canonical isomorphism $\Gamma^\infty(TX \otimes \mathbb{C}) \to \Omega^{d-1}(X; L \otimes \mathbb{C})$, $v \mapsto \iota(v)\, \mathrm{dvol}_X$.

Remark 3.4. Our current operator is $\mathbb{C}$-linear in the first factor of $\Gamma^\infty(E) \otimes_{\mathbb{R}} \Gamma^\infty(E)$ but $\mathbb{C}$-anti-linear in the second factor. Alternatively, from the viewpoint of the next subsection where the transcription to kernels will be made, the current operator is a $\mathbb{C}$-bilinear mapping $\Gamma^\infty(E) \otimes_{\mathbb{C}} \Gamma^\infty(E^*) \to \Gamma^\infty(TX \otimes \mathbb{C})$. The two viewpoints are related via the anti-linear bijection $\Gamma^\infty(E) \to \Gamma^\infty(E^*)$, $\varphi \mapsto h(\varphi\,, \cdot)$.

By the principle of (2.3), the exterior derivative of the differential form $j(\psi, \varphi)$ corresponds to the divergence of the vector field $v(\psi, \varphi)$. From (3.8) one therefore has the following consequence, which will be put to multiple use in Sect. 4.

Proposition 3.5. *The current vector field $v(\psi, \varphi)$ has divergence*

$$\operatorname{div} v(\psi, \varphi) = \mathrm{i}h(\varphi\,, D\psi) - \mathrm{i}h(D^\dagger \varphi\,, \psi)\ .$$

In particular, if ψ and φ are eigensections with complex conjugate eigenvalues, i.e.,

$$D\psi = \lambda\psi\ , \quad D^\dagger\varphi = \bar{\lambda}\varphi \qquad (\lambda \in \mathbb{C})\ ,$$

then $v(\psi, \varphi)$ is divergenceless.

To prepare the next step, note that if $\langle v, \xi\rangle \equiv \iota(v)\xi$ denotes the function which is obtained by contracting the vector field v with the 1-form ξ, then the current vector field $v(\psi, \varphi)$ has a more direct definition from (3.7) as

$$\int_X \langle v(\psi, \varphi), A'\rangle \,\mathrm{dvol}_X = \frac{d}{ds}(\varphi\,, D_{\nabla + \mathrm{i}sA'}\psi)\Big|_{s=0}\ . \tag{3.9}$$

Example 3.6. Specializing to the case of a Dirac-type operator $D = c(\mathrm{d}x^i)\nabla_{\partial/\partial x^i}$ one obtains the formula

$$\langle v(\psi, \varphi), A'\rangle = h(\varphi\,, \mathrm{i}c(A')\psi)\ .$$

3.3. **Transcription to kernels.** Our next step is to transcribe the above to the language of kernels. Let $E \boxtimes E^*$ denote the exterior tensor product of E with its dual bundle. $E \boxtimes E^*$ is a bundle over the product manifold $X \times X$, where the fiber over $(x, y) \in X \times X$ is the space of linear transformations $E_x \otimes E_y^* \cong \mathrm{Hom}(E_y\,, E_x)$. A section $k(\cdot\,, \cdot) \in \Gamma^\infty(E \boxtimes E^*)$ gives rise to a linear operator

$$K\ :\ \Gamma_c^\infty(E) \longrightarrow \Gamma^\infty(E)\ , \quad \psi \mapsto K\psi\ , \quad (K\psi)(x) := \int_X k(x, \cdot)\psi \,\mathrm{dvol}_X\ . \tag{3.10}$$

Here the integrand $k(x, \cdot)\psi$ is the E_x-valued function whose value at y is obtained by applying the linear transformation $k(x, y) \in \mathrm{Hom}(E_y\,, E_x)$ to the vector $\psi(y) \in E_y$. When $k \in \Gamma_c^\infty(E \boxtimes E^*)$, it is well known that K is a trace-class operator in $L^2(X, E)$ and that

$$\operatorname{Tr} K = \int_X \operatorname{tr}_{E_x} k(x, x) \,\mathrm{dvol}_X(x)\ . \tag{3.11}$$

Note that the composite operators DK and KD have the kernels

$$(DK)(x, y) = D_x k(x, y)\ , \quad (KD)(x, y) = D_y^{\mathrm{t}} k(x, y)\ . \tag{3.12}$$

The notation with subscript here means that the differential operator $D \equiv D_x$ acts on the kernel $k(x, y)$ as a function of its first variable. $D^{\mathrm{t}} \in \mathrm{Diff}(E^*)$ is the operator induced from D by dualization from $\Gamma^\infty(E)$ to $\Gamma^\infty(E^*)$, i.e., $D^{\mathrm{t}} h(\psi, \cdot) = h(D^\dagger\psi, \cdot)$.

Now, adapting the previous construction of (3.9) to the present situation, we are going to produce a vector field from a kernel $k \in \Gamma_c^\infty(E \boxtimes E^*)$. This leads us to our second definition of current operator.

Definition 3.7. The current operator on kernels is the linear mapping

$$\Gamma_c^\infty(E \boxtimes E^*) \longrightarrow \Gamma^\infty(TX \otimes \mathbb{C})\ , \quad k \mapsto v(k)\ ,$$

where the current vector field $v(k)$ is determined by the equation

$$\int_X \langle v(k), A'\rangle \,\mathrm{dvol}_X = \frac{d}{ds} \operatorname{Tr}\left(D_{\nabla + \mathrm{i}sA'} K\right)\Big|_{s=0}$$

for all test forms $A' \in \Omega_c^1(X)$. (Again, the vector field $v(k)$ continues to exist even when the assumption of compact support for k is dropped.)

If f is any compactly supported test function and $A' = \mathrm{d}f$, then by the same computation as before,

$$\int_X f \operatorname{div} v(k) \, \mathrm{dvol}_X = -\mathrm{i}\operatorname{Tr}([D, f]K) \, .$$

Since the trace is cyclic, the right-hand side can also be written as $\mathrm{i}\operatorname{Tr}(f[D, K])$. Thus, if the linear operator K commutes with D, the current vector field $v(k)$ is divergenceless. More generally, by inserting the expressions (3.12) for the kernels of DK and KD, one obtains

Proposition 3.8.

$$\operatorname{div}(v(k))(x) = \mathrm{i}\, \mathrm{tr}_{E_x} \left(D_x k(x, y) - D_y^{\mathrm{t}} k(x, y) \right) \Big|_{y=x} \, .$$

Remark 3.9. If our kernel $k \in \Gamma^\infty(E \boxtimes E^*)$ satisfies $D_x k(x, y) = \lambda\, k(x, y)$ and $D_y^{\mathrm{t}} k(x, y) = \mu\, k(x, y)$ for $\lambda\,, \mu \in \mathbb{C}$, then the formula of Prop. 3.8 reduces to

$$\operatorname{div}(v(k))(x) = (\lambda - \mu)\, \mathrm{tr}_{E_x} k(x, x) \, . \tag{3.13}$$

Now let there be *two* kernels $k_1, k_2 \in \Gamma_c^\infty(E \boxtimes E^*)$, with associated linear operators K_1 and K_2 . By iterating the procedure above, we associate to them a bi-vector field $\Sigma(K_1, K_2)$ as follows. A bi-vector field determines a bilinear functional on test forms $A', A'' \in \Omega_c^1(X)$ by integration over $X \times X$. Comparing this with the bilinear functional obtained from $\operatorname{Tr}(D_{\nabla + \mathrm{i}sA'} K_1 D_{\nabla + \mathrm{i}tA''} K_2)$ by linearization in s and t , we define $\Sigma(K_1, K_2)$ to be the bi-vector field that makes the two functionals equal:

$$\begin{aligned} &\int_X \int_X \big\langle \Sigma(K_1, K_2)(x, y) \, , (A'_x \, , A''_y) \big\rangle \, \mathrm{dvol}_X(x) \, \mathrm{dvol}_X(y) \\ &= \frac{d^2}{ds dt} \operatorname{Tr} \left(D_{\nabla + \mathrm{i}sA'} K_1 D_{\nabla + \mathrm{i}tA''} K_2 \right) \Big|_{s=t=0} \, , \end{aligned} \tag{3.14}$$

for all A', A''. Depending on the point of view, $\Sigma(K_1, K_2)$ is a bi-vector field or a vector field on $X \times X$. It has the obvious symmetry

$$\langle \Sigma(K_1, K_2), (A', A'') \rangle = \langle \Sigma(K_2 \, , K_1), (A'', A') \rangle \, .$$

3.4. **Conductivity bi-vector field.** Let us now specialize the previous formulas to the case of resolvents, $K_1 = (D - \lambda)^{-1}$ and $K_2 = (D - \lambda')^{-1}$, whose kernels k_1 and k_2 are not smooth. Therefore we emphasize that the formulas are completely local; in order for them to hold it is not necessary that the kernels be smooth everywhere. In fact, $\Sigma(K_1, K_2)(x, y)$ already exists if k_1 is smooth in the point $(x, y) \in X \times X$ and k_2 is smooth in the point (y, x).

We now rely on some input from the physics literature [1]. Starting from the formalism of second quantization for many-fermion systems, and specializing to the case of non-interacting particles with Fermi energy E_F , the Kubo theory of linear response yields the following formula for the bi-vector field of the electrical conductivity σ. We here take this formula for granted and do not discuss its origin in linear-response theory.

Definition 3.10. With a pair of complex numbers λ and λ' not in the spectrum of D, associate a bi-vector field $\sigma_{\lambda,\lambda'}$ by

$$\begin{aligned} \sigma_{\lambda,\lambda'} \;&=\; \Sigma\left((D - \lambda)^{-1}, (D - \lambda')^{-1}\right) \\ &-\; \tfrac{1}{2}\Sigma\left((D - \lambda)^{-1}, (D - \lambda)^{-1}\right) - \tfrac{1}{2}\Sigma\left((D - \lambda')^{-1}, (D - \lambda')^{-1}\right) \\ &+\; \tfrac{1}{2} \int_{\lambda'}^{\lambda} \Sigma\left((D - \mu)^{-1}, (D - \mu)^{-2}\right) - \Sigma\left((D - \mu)^{-2}, (D - \mu)^{-1}\right) d\mu \, , \end{aligned}$$

where the integral is along any contour in the domain of holomorphicity of the resolvent kernel $(D-\mu)^{-1}$ and its derivative $(D-\mu)^{-2}$. Then the d.c. (or static) linear-response electrical conductivity at the Fermi energy $E \in \mathbb{R}$ is given by

$$\sigma_E := \lim_{\epsilon \to 0+} \sigma_{E+\mathrm{i}\epsilon, E-\mathrm{i}\epsilon} \, .$$

By the same argument that gave Proposition 3.8 and equation (3.13), this bi-vector field σ_E satisfies postulate (2.4) of Definition (2.2). `What is less clear, however, is whether` σ_E `is smooth on the diagonal` $x = y$. `ML says we can get enough regularity for the symmetric part of` σ_E `in order for the proof of Proposition 2.4 to go through.`

4. Dirac operator on a manifold with cylindrical contacts

In this section we study the quantum mechanical scattering problem on a d-dimensional manifold M with cylindrical ends (interpreted as electrical contacts), where the incoming and outgoing waves are the asymptotic running waves on the cylinders. The dynamics is determined by a generalized Dirac operator, $\mathscr{D}$. In the language of standard scattering theory the operator $\mathscr{D}_0$ on the cylinders is the free part of the Hamiltonian and the unperturbed states are its eigenfunctions satisfying certain boundary conditions. Scattering arises from attaching the cylinders to M, and is determined by the operator $\mathscr{D}_M$ on M.

One complication in this setting stems from the fact that the free Hamiltonian $\mathscr{D}_0$ and the scattering part $\mathscr{D}_M$ do not operate in the same Hilbert space. Fortunately, there exists a scattering theory of operators acting in different Hilbert spaces (cf. [11]), and this theory applies here. The Møller operators of our problem exist and are complete, so they provide a unitary equivalence between the absolute continuous part of $\mathscr{D} := \mathscr{D}_M \cup \mathscr{D}_0$ and $\mathscr{D}_0$ [10, 6]. We will use the Lippmann-Schwinger equation together with an asymptotic expansion of the resolvent kernel to express the sum of scattering probabilities (between channels of incoming and outgoing waves in the cylinders) as a double integral over the conductivity bi-vector field σ.

Our calculation in spirit follows that of Baranger and Stone [1], who arrived at the same result for Schrödinger operators. Although we prove the result for the special case of Dirac dynamics, it can be expected to hold in much wider generality.

4.1. **Setup.** Given a Hermitian vector bundle E over a compact Riemannian manifold M with boundary $Y = \partial M$, let there be a Dirac-type operator $\mathscr{D}_M$ acting on the sections of E. We assume that $\mathscr{D}_M$ is formally self-adjoint and on restricting to a collar $[-\varepsilon, 0] \times Y$ of M decomposes as

$$\mathscr{D}_M\big|_{[-\varepsilon,0]\times Y} =: \mathscr{D}_0 = \gamma \left(\frac{d}{dr} + A \right) . \tag{4.1}$$

Here $r : [-\varepsilon, 0] \times Y \to [-\varepsilon, 0]$ is the coordinate function projecting on the first factor. γ is the normal component of the symbol of $\mathscr{D}_0$, i.e.,

$$\gamma = [\mathscr{D}_0 \, , r] = c(\mathrm{d}r) \, , \tag{4.2}$$

and γA is the transversal part of $\mathscr{D}_0$. The relations

$$\gamma^2 = -\mathbb{1} \ , \quad \gamma^* = -\gamma \ , \quad A = A^\dagger \ , \quad \gamma A + A\gamma = 0 \tag{4.3}$$

are assumed to hold.

From (4.1) the operator $\mathscr{D}_0$ extends naturally to the cylinder $\mathbb{R}_+ \times Y$ and hence we get a Dirac-type operator $\mathscr{D} = \mathscr{D}_M \cup \mathscr{D}_0$ on the manifold X obtained by gluing M and $\mathbb{R}_+ \times Y$ along the common boundary,

$$X = M \cup_{\partial M} (\mathbb{R}_+ \times Y) \ . \tag{4.4}$$

Since X is complete, $\mathscr{D}$ is essentially self-adjoint (Wolf [13], Chernoff [5]). The scattering problem for $\mathscr{D}$ on X was studied by Guillopé [6] and W. Müller [10]. The new information conveyed in the present paper is the relation between scattering and the electrical conductance. For the convenience of the reader, we make an attempt to give a self-contained exposition.

In the scattering problem to be studied, $\mathscr{D}$ will be viewed as a perturbation of $\mathscr{D}_0$. To define the unperturbed problem governed by $\mathscr{D}_0$ we have yet to impose boundary conditions at $\partial(\mathbb{R}_+ \times Y) = \{0\} \times Y$. (As a general reference for boundary value problems for Dirac-type operators we refer to the book of Booß–Bavnbek and Wojciechowski [2]). We fix a Lagrangian subspace[1] $V \subset \ker A$ and define the spectral projector

$$P_+ := 1_{(0,\infty)}(A) + P_V \,, \tag{4.5}$$

where $1_{(0,\infty)}$ is the characteristic function of the set $(0, \infty)$. With this we impose generalized Atiyah–Patodi–Singer boundary conditions:

$$\mathrm{domain}(\mathscr{D}_0) := \{v \in L^2 \mid \mathscr{D}_0 v \in L^2,\ P_+ v\Big|_{r=0} = 0\}\,. \tag{4.6}$$

Since Y is compact and A is elliptic, the spectrum of A is discrete. We choose an orthonormal basis $(\varphi_n)_{n\in\mathbb{N}}$ of $\mathrm{im}P_+$ with

$$A\varphi_n = a_n\varphi_n\,, \quad a_n \geq 0\,. \tag{4.7}$$

By virtue of the last relation in (4.3), $\gamma\varphi_n$ is an eigenvector of A with eigenvalue $-a_n$. It follows from this and the Lagrangian property of V in (4.5) that

$$\gamma P_+ \gamma^* = I - P_+ \,, \tag{4.8}$$

and hence $(\gamma\varphi_n)_{n\in\mathbb{N}}$ is an orthonormal basis of $\mathrm{im}(I - P_+) = \ker P_+$.

It will be convenient to have a name for the set of positive eigenvalues:

$$S := \{a_n \mid n \in \mathbb{N}\} \setminus \{0\}\,. \tag{4.9}$$

In S each value a_n is counted once, regardless of degeneracies. This distinguishes the sum $\sum_n$ over eigenmodes (of either sign and zero) from the summation $\sum_{a\in S}$ over positive values appearing in the spectrum.

In the next step, we turn to the $(\varphi, \gamma\varphi)$-basis and write $\mathscr{D}_0$ as a direct sum of operators D_n acting in $L^2(\mathbb{R}_+, \mathrm{span}(\varphi, \gamma\varphi))$:

$$\mathscr{D}_0 = \bigoplus_{n\in\mathbb{N}} D_n\,, \tag{4.10}$$

with

$$D_n = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \left[\frac{d}{dr} + \begin{pmatrix} a_n & 0 \\ 0 & -a_n \end{pmatrix} \right]. \tag{4.11}$$

Thus, each D_n operates on complex two-component fields

$$\{r \mapsto v_n(r)\} \in \mathrm{domain}(D_n)\,, \quad v_n(r) = \begin{pmatrix} \alpha(r) \\ \beta(r) \end{pmatrix}\,,$$

and for the greater part of this section we will be interested in such fields $v_n(r)$ only. In order to avoid introducing new symbols, we will later use the same symbol for sections in the domain of $\mathscr{D}_0$, but this change of meaning will be indicated by explicitly giving the full dependence on $(r, \xi) \in \mathbb{R}_+ \times Y$:

$$v_n(r) = \begin{pmatrix} \alpha(r) \\ \beta(r) \end{pmatrix} \quad \text{will become} \quad v_n(r,\xi) := \alpha(r)\varphi_n(\xi) + \beta(r)\gamma\varphi_n(\xi)\,. \tag{4.12}$$

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[1] This means that $V^\perp = \gamma V$. The existence of V follows from the Cobordism Theorem (Palais [12, Chap. XVII]; cf. also Lesch [9]).

4.2. **Analytic continuation of the scattering states.** We denote the eigenfunctions of D_n by ψ_n^0. The superscript indicates that these are solutions to the free Dirac operator $\mathscr{D}_0$. In the φ-basis the boundary condition (4.6) requires the upper component of ψ_n^0 to be zero at $r = 0$. An eigenvector $\psi_n^0(\cdot\,;\lambda)$ satisfying

$$(\mathscr{D}_0 - \lambda)\psi_n^0(\cdot\,;\lambda) = 0$$

is

$$\begin{aligned} \psi_n^0(r\,;\lambda) &= 2^{-1/2}\begin{pmatrix} \sin(k_n(\lambda)r) \\ \lambda^{-1}a_n\sin(k_n(\lambda)r) + \lambda^{-1}k_n(\lambda)\cos(k_n(\lambda)r) \end{pmatrix}, \\ k_n(\lambda) &:= \sqrt{\lambda^2 - a_n^2}\,, \end{aligned} \tag{4.13}$$

where k_n is called the wave number. $\psi_n^0(r\,;\lambda)$ is an analytic (multivalued!) function of the complex parameter λ, and has the physical interpretation of a standing wave. Please be advised that our choice of normalization for ψ_n^0 is convenient, but not standard; we will get back to this point in Remark 4.5 below.

Definition 4.1. We choose $\sqrt{} : \mathbb{C}\setminus\mathbb{R}_+ \to \mathbb{C}$, $z \mapsto \sqrt{z}$, to be the principal branch of the square root given by $\operatorname{Im}\sqrt{z} > 0$.

We now describe the analytic continuation of $\psi_n^0(r\,;\lambda)$ in terms of the Riemann surface of the functions $\sqrt{\lambda^2 - a^2}$ for $a \in S$. Since there exist infinitely many values $a \in S$, to get a true Riemann surface with only countably many sheets[2] one has to impose a restriction for large a. More concretely, let

$$\mathbb{C}^{\mathbb{N}} := \{(z_n)_{n\in\mathbb{N}} \mid z_n \in \mathbb{C}\} \tag{4.14}$$

be the space of complex sequences equipped with the topology of uniform convergence. Put

$$\Sigma := \left\{(z\,,\{w_a\}_{a\in S}) \;\middle|\; \begin{matrix} z \in \mathbb{C}\,,\ w_a^2 = z^2 - a^2 \text{ for } a \in S\,, \\ \operatorname{Im} w_a > 0 \text{ for } a \text{ large enough} \end{matrix} \right\} \subset \mathbb{C}^{\mathbb{N}}. \tag{4.15}$$

Then Σ is a Riemann surface with the following properties:

(1) The projection $\pi : \Sigma \to \mathbb{C}$, $(z\,,\{w_a\}_{a\in S}) \mapsto z$ is a branched cover with countably many sheets and ramification locus $S \cup (-S)$.

(2) $W_a : \Sigma \to \mathbb{C}$, $(z\,,\{w_b\}_{b\in S}) \mapsto w_a$ are holomorphic functions satisfying

$$W_a(\Lambda)^2 = \pi(\Lambda)^2 - a^2\,, \quad a \in S\,, \tag{4.16}$$

and, for fixed $\Lambda \in \Sigma$, we have $\operatorname{Im} W_a(\Lambda) > 0$ when a is large enough.

(3) The group of deck transformations of $(\Sigma\,,\mathbb{C})$ is commutative and is generated by elements τ_a of order 2. More precisely,

$$\tau_a(z\,,\{w_b\}_{b\in S}) = (z\,,\{\widetilde{w}_b\}_{b\in S}) \quad \text{where} \quad \widetilde{w}_b = \begin{cases} w_b\,, & b \neq a\,, \\ -w_a\,, & b = a\,. \end{cases} \tag{4.17}$$

In other words, by the generator τ_a the functions W_b are pulled back to

$$\tau_a^* W_b = \begin{cases} W_b\,, & b \neq a\,, \\ -W_a\,, & b = a\,. \end{cases} \tag{4.18}$$

We will, by slight abuse of notation, write τ_n instead of τ_{a_n}.

(4) For $\Lambda\,,\Lambda' \in \Sigma$ to be equal it is necessary and sufficient that

$$\pi(\Lambda) = \pi(\Lambda') \quad \text{and} \quad \forall a \in S:\ W_a(\Lambda) = W_a(\Lambda')\,.$$

[2] Note that for each $z \in \mathbb{C}$ there are uncountably many sequences $\{w_a\}_{a\in S}$ with $w_a^2 = z^2 - a^2$.

(5) Putting

$$\overline{(z\,,\{w_a\}_{a\in S})} := (\overline{z}\,,\{-\overline{w}_a\}_{a\in S}) \tag{4.19}$$

extends the operation of complex conjugation to a diffeomorphism $\Sigma \to \Sigma$, $\Lambda \mapsto \overline{\Lambda}$ with the properties

$$\text{(i)} \quad \pi(\overline{\Lambda}) = \overline{\pi(\Lambda)}\ , \quad \text{(ii)} \quad W_a(\overline{\Lambda}) = -\overline{W_a(\Lambda)}\,. \tag{4.20}$$

(6) The function $\lambda \mapsto \psi_n^0(r\,;\lambda)$ extends as a meromorphic function to the Riemann surface Σ.

Although $\Lambda \in \Sigma$ is not a complex number and its square is not defined, we will mostly employ the suggestive notation $\sqrt{\Lambda^2 - a^2}$ for the function $W_a(\Lambda)$.

Remark 4.2. Guillopé [6, Sect. 7C] uses a slightly different Riemann surface Σ^s. On Σ^s the functions $\sqrt{\Lambda \pm a}$ exist individually. Guillopé uses the normalization $\operatorname{Im}\sqrt{\Lambda \pm a} > 0$ for a large enough. Apart from the fact that for $\pi(\Lambda) \in \mathbb{R}$ this can be fulfilled only with equality $\operatorname{Im}\sqrt{\Lambda + a} = 0$, there is a serious problem with this normalization. In fact, it sometimes contradicts $\operatorname{Im}\sqrt{\Lambda^2 - a^2} > 0$. Thus on Σ^s we do not always have $\operatorname{Im}\sqrt{\Lambda - a}\sqrt{\Lambda + a} > 0$ for a large enough. As a consequence Σ^s is not a branched cover of Σ. If one modifies the normalization of Σ^s to $\operatorname{Im}\sqrt{\Lambda + a} > 0$, $\operatorname{Im}\sqrt{\Lambda - a}\sqrt{\Lambda + a} > 0$, for a large enough, and this is apparently the normalization Guillopé wants to work with [6, p. 159, second paragraph], then Σ^s is naturally a branched cover of our surface Σ. Nevertheless, since only the functions $\sqrt{\Lambda^2 - a^2}$ are needed (cf. also [6, Prop. 7.7]) we prefer to work with Σ.

If $a = a_n \in S$ we set $k_n(\Lambda) := W_a(\Lambda)$ (although, as we emphasize, the functions W_a are labelled by elements of S and not by modes). $\psi_n^0(r\,;\Lambda)$ is now a meromorphic function of $\Lambda \in \Sigma$ satisfying

$$(D_n - \pi(\Lambda))\psi_n^0(r\,;\Lambda) = 0\ . \tag{4.21}$$

The domain

$$\mathrm{FP} := \mathbb{C} \setminus \big((-\infty, -\inf S] \cup [\inf S, \infty)\big) \tag{4.22}$$

is identified with an open subset of Σ, the *physical sheet.*

For points $E \in \mathbb{R} \setminus (S \cup -S)$ we introduce the following notation:

$$E_\pm := \lim_{\varepsilon \to 0+} E \pm \mathrm{i}\varepsilon\ , \tag{4.23}$$

where the limit is taken in Σ. In other words, lying over $E \in \mathbb{R} \setminus (S \cup -S)$, the limit $E_\pm \in \Sigma$ is the point which is obtained by taking the *limit in* Σ when approaching E on the physical sheet from the upper/lower half plane. Since

$$\lim_{\varepsilon \to 0+} \sqrt{(E + \mathrm{i}\varepsilon)^2 - a_n^2} = \begin{cases} \lim\limits_{\varepsilon \to 0+} \sqrt{(E - \mathrm{i}\varepsilon)^2 - a_n^2}\ , & |E| < a_n\ , \\ -\lim\limits_{\varepsilon \to 0+} \sqrt{(E - \mathrm{i}\varepsilon)^2 - a_n^2}\ , & |E| > a_n\ , \end{cases} \tag{4.24}$$

by our definition of square root $\sqrt{\ }$, we have

$$\begin{aligned} \sqrt{(E_+)^2 - a_n^2} &= \begin{cases} \mathrm{i}\sqrt[+]{(a_n^2 - E^2)}\ , & |E| < a_n\ , \\ \sqrt[+]{(E^2 - a_n^2)}\ , & |E| > a_n\ , \end{cases} \\ &= \begin{cases} \sqrt{(E_-)^2 - a_n^2}\ , & |E| < a_n\ , \\ -\sqrt{(E_-)^2 - a_n^2}\ , & |E| > a_n\ , \end{cases} \\ &= -\overline{\sqrt{(E_-)^2 - a_n^2}}\ . \end{aligned} \tag{4.25}$$

Here $\sqrt{_+ x}$ denotes the positive square root of $x \geq 0$. From $W_a(E_\pm) \equiv \sqrt{(E_\pm)^2 - a_n^2}$ and the definition (4.19) we find as a consequence

$$\overline{E_\pm} = E_\mp \; . \tag{4.26}$$

For present use, note that as a special case of (4.18) we have

$$W_{a_n}(\Lambda) \equiv k_n(\Lambda) = -k_n(\tau_n \Lambda) \; .$$

4.3. **Running waves.** The standing-wave solutions ψ_n^0 in (4.13) can be separated into purely exponential functions of the longitudinal cylinder coordinate r like this: for $\Lambda \in \Sigma$ consider

$$\phi_n^0(r\,;\Lambda) := 2^{-1/2} \begin{pmatrix} 1 \\ (a_n + \mathrm{i}k_n(\Lambda))/\pi(\Lambda) \end{pmatrix} \exp\left(\mathrm{i}k_n(\Lambda) r\right) , \tag{4.27}$$

which is easily seen to be an eigenfunction of $\mathscr{D}_0$ with eigenvalue $\pi(\Lambda)$ but obviously violates the boundary conditions. Using the deck transformation τ_n in (4.17) and $k_n(\tau_n\Lambda) = -k_n(\Lambda)$, the true eigenfunction ψ_n^0 (which does satisfy the boundary conditions) extends from FP to Σ as the linear combination

$$\psi_n^0(r\,;\Lambda) = \frac{1}{2\mathrm{i}} \left(\phi_n^0(r\,;\Lambda) - \phi_n^0(r\,;\tau_n\Lambda) \right) \; . \tag{4.28}$$

To interpret this decomposition of ψ_n^0, observe that the time-dependent free Dirac equation is $(\mathrm{i}\partial_t - \mathscr{D}_0)v = 0$, so that ϕ_n^0 gives rise to a time-dependent solution

$$(r,t) \mapsto \mathrm{e}^{-\mathrm{i}\pi(\Lambda)t} \phi_n^0(r\,;\Lambda) \,.$$

If $E_+ \in \Sigma$ lies over $E \in \mathbb{R}$ with $|E| > a_n$, then the phase function

$$(r,t) \mapsto k_n(E_+) r - \pi(E_+) t$$

is real, and its zero locus moves with growing values of t to growing values of r. Thus, the time-dependent solution given by ϕ_n^0 has the physical meaning of an *outgoing* wave in that case. By the same token, $\phi_n^0(\cdot\,;\tau_n E_+)$ gives rise to an *incoming* wave. We therefore refer to $\phi_n^0(\cdot\,;\Lambda)$ and $\phi_n^0(\cdot\,;\tau_n\Lambda)$ summarily as running waves (of outgoing resp. incoming type). Note that by the definition of the physical sheet, the outgoing waves $\phi_n^0(\cdot\,;\lambda)$ for $\lambda \in$ FP and $\operatorname{Im}\lambda \neq 0$ are square-integrable on $\mathbb{R}_+$ while the incoming waves $\phi_n^0(\cdot\,;\tau_n\lambda)$ are not.

4.4. **Orthogonality relations on the cylinder.** Prop. 3.5 says that for two eigensections ψ and φ with eigenvalues λ resp. $\bar\lambda$ the current vector field $v(\psi,\varphi)$ is divergenceless. This circumstance gives rise to a set of fixed-energy orthogonality relations by integration over a $(d-1)$-cycle of X. We will make this explicit for the running waves, where the integration will be over cross sections of the cylinder.

First of all, we write out the running waves (4.27) with full coordinate dependence as anticipated in (4.12):

$$\phi_n^0(r,\xi\,;\Lambda) = 2^{-1/2}\big(\varphi_n(\xi) + \pi(\Lambda)^{-1}(a_n + \mathrm{i}k_n(\Lambda))\gamma\varphi_n(\xi)\big)\,\mathrm{e}^{\mathrm{i}k_n(\Lambda)r}. \tag{4.29}$$

Then, fixing a pair of positive integers m,n we pick any two points $\Lambda_1\,,\Lambda_2$ of the Riemann surface Σ with $\pi(\Lambda_{1,2}) \neq 0$ and consider the integral

$$I_{m,n}(r\,;\Lambda_1\,,\Lambda_2) := \int_Y h\left(\phi_m^0(r,\xi\,;\Lambda_1), \mathrm{i}\gamma\phi_n^0(r,\xi\,;\Lambda_2)\right) \mathrm{dvol}_Y(\xi) \;, \tag{4.30}$$

where $\mathrm{dvol}_Y = \iota(\partial_r)\,\mathrm{dvol}_X$. From Example 3.6, and since $\gamma = c(\mathrm{d}r)$, this can also be written as

$$I_{m,n}(r\,;\Lambda_1\,,\Lambda_2) = \int_Y v\left(\phi_n^0(\cdot\,;\Lambda_2), \phi_m^0(\cdot\,;\Lambda_1)\right)\Big|_r \;. \tag{4.31}$$

We remind the reader that, if $Y \subset X$ is a $(d-1)$-dimensional submanifold, then by the integral of a vector field v over Y we mean $\int_Y v = \int_Y \iota(v)\,\mathrm{dvol}_X$.

Furthermore, since $(\pi(\Lambda_1) - \mathscr{D}_0)\phi^0_m(\cdot\,;\Lambda_1) = 0$ and $(\pi(\Lambda_2) - \mathscr{D}_0)\phi^0_n(\cdot\,;\Lambda_2) = 0$, the second statement of Prop. 3.5 says that $v(\phi^0_n(\cdot\,;\Lambda_2), \phi^0_m(\cdot\,;\Lambda_1))$ is divergenceless if $\overline{\pi(\Lambda_1)} = \pi(\Lambda_2)$. In that case, the integral (4.31) is constant on the homology class of Y; in particular it is independent of r.

Substituting (4.29) into (4.30) we find for any $\Lambda_1, \Lambda_2 \in \Sigma$ that

$$I_{m,n}(r\,;\Lambda_1\,,\Lambda_2) = I_{m,n}(0\,;\Lambda_1\,,\Lambda_2)\,\mathrm{e}^{-\mathrm{i}\overline{k_m(\Lambda_1)}r+\mathrm{i}k_n(\Lambda_2)r}\,. \tag{4.32}$$

Since the φ_n constitute an orthonormal system, the integral $I_{m,n}(0\,;\Lambda_1\,,\Lambda_2)$ vanishes for $m \neq n$. For $m = n$ insertion of (4.29) into (4.30) gives

$$I_{n,n}(0\,;\Lambda_1\,,\Lambda_2) = \frac{\overline{k_n(\Lambda_1)} + \mathrm{i}a_n}{2\overline{\pi(\Lambda_1)}} + \frac{k_n(\Lambda_2) - \mathrm{i}a_n}{2\pi(\Lambda_2)}\,. \tag{4.33}$$

4.4.1. *The case* $\overline{\pi(\Lambda_1)} = \pi(\Lambda_2)$. In this case there exist the two possibilities

$$\overline{k_n(\Lambda_1)} = \pm k_n(\Lambda_2)\,, \tag{4.34}$$

and the expression (4.33) together with (4.20) yields the following statement.

Proposition 4.3. *Let* $\overline{\pi(\Lambda_1)} = \pi(\Lambda_2) \neq 0$. *Then* $I_{m,n}(r\,;\Lambda_1\,,\Lambda_2)$ *is independent of* r *and we have*

$$I_{m,n}(r\,;\Lambda_1\,,\Lambda_2) = \delta_{m,n}\begin{cases} 0\,, & \overline{k_n(\Lambda_1)} = -k_n(\Lambda_2), \\ k_n(\Lambda_2)/\pi(\Lambda_2)\,, & \overline{k_n(\Lambda_1)} = k_n(\Lambda_2)\,. \end{cases} \tag{4.35}$$

In particular, if $\overline{\Lambda_1} = \Lambda_2$ *then* $I_{m,n}(r\,;\Lambda_1\,,\Lambda_2) = 0$ *for all* $m\,,n$.

We specialize even further to the case where $\Lambda_{1,2}$ are two points $E_\pm \in \Sigma$ lying over the same $E \in \mathbb{R}$. By (4.25) and (4.26) we then arrive at the following result.

Proposition 4.4. *Let* $E \in \mathbb{R} \setminus \{\pm a_m\,, \pm a_n\,, 0\}$. *Then*

$$I_{m,n}(r\,;E_\pm, E_\mp) = 0\,, \tag{4.36}$$

$$I_{m,n}(r\,;E_\pm, E_\pm) = \delta_{m,n}\begin{cases} 0\,, & |E| < a_n\,, \\ \pm\sqrt{_+(1 - a_n^2/E^2)}\,, & |E| > a_n\,. \end{cases} \tag{4.37}$$

Remark 4.5. Here a comment on normalization is in order. If we had adopted the standard (unit flux) normalization convention of scattering theory, we would have obtained $I_{m,n}(r\,;E_\pm, E_\pm) = \pm\delta_{m,n}$. We did not opt for this choice of normalization here, as it would have made the analytic properties (in λ) of the scattering waves more complicated. The price we will have to pay is that the expression for the conductance will not emerge in the familiar (Landauer-Büttiker) form.

4.5. **Lippmann-Schwinger equation.** Now we turn to the full Dirac operator $\mathscr{D}$ and its eigensections $x \mapsto \psi_n(x\,;\Lambda)$, where x runs through $X = M \cup_{\partial M} (\mathbb{R}_+ \times Y)$. As was mentioned in the introduction to this section, compared to standard scattering theory we are facing the complication that the full Hamiltonian $\mathscr{D} = \mathscr{D}_M \cup \mathscr{D}_0$ and the free part $\mathscr{D}_0$ do not act in the same Hilbert space; $\mathscr{D}_0$ acts in $L^2(\mathbb{R}_+ \times Y, E)$ whereas $\mathscr{D}$ acts in $L^2(X, E)$. While we tacitly view $L^2(\mathbb{R}_+ \times Y, E)$ as a subspace of $L^2(X, E)$, the inclusion $L^2(\mathbb{R}_+ \times Y, E) \hookrightarrow L^2(X, E)$ does not preserve smoothness. To mend this, we choose on the semi-infinite cylinder $\mathbb{R}_+ \times Y$ a smooth cutoff function $\chi : \mathbb{R}_+ \times Y \to \mathbb{R}$ with

$$\chi(x) = \begin{cases} 0\,, & r(x) < r_1\,, \\ 1\,, & r(x) > r_2\,, \end{cases} \tag{4.38}$$

where $0 < r_1 < r_2 < 1$ are fixed. Letting $M_\chi : L^2(\mathbb{R}_+ \times Y, E) \to L^2(X, E)$ be the operation of point-wise multiplication by χ, we then define the Møller operators

$$\mathscr{W}_\pm(\mathscr{D}, \mathscr{D}_0) = \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}t\mathscr{D}} M_\chi \, \mathrm{e}^{-\mathrm{i}t\mathscr{D}_0} \,. \tag{4.39}$$

It follows from the results of Guillopé [6] that the wave operators $\mathscr{W}_\pm$ exist and are complete. They establish a unitary equivalence of $\mathscr{D}_0$ and the absolutely continuous part of $\mathscr{D}$. Furthermore, Guillopé [6] proved the following important result. To state it, we need the spaces $L^2_{\mathrm{comp}}(X, E)$, $L^2_{\mathrm{loc}}(X, E)$ of compactly supported L^2-sections resp. local L^2-sections of E. These spaces have natural locally convex topologies and we denote by $\mathscr{L}_s(L^2_{\mathrm{comp}}, L^2_{\mathrm{loc}})$ the space of continuous linear operators between L^2_{comp}, L^2_{loc} equipped with the topology of point-wise convergence.

Proposition 4.6. *The resolvent $(\mathscr{D} - \lambda)^{-1}$ of $\mathscr{D}$ considered as a function on the physical sheet with values in $\mathscr{L}_s(L^2_{\mathrm{comp}}, L^2_{\mathrm{loc}})$ extends meromorphically to Σ.*

We denote this meromorphic extension by $(\mathscr{D} - \Lambda)^{-1}, \Lambda \in \Sigma$. More concretely, we may think of $(\mathscr{D} - \Lambda)^{-1}$ as an integral operator whose kernel is obtained by meromorphic continuation of the kernel of $(\mathscr{D} - \lambda)^{-1}$.

We can now set up the Lippmann-Schwinger equations for this problem. For the following definition, note that $[\mathscr{D}, \chi] = \gamma\chi'$ where $\chi' = \partial\chi/\partial r$.

Definition 4.7. For $\Lambda \in \Sigma$ put

$$\psi_n(\,\cdot\,;\Lambda) := M_\chi \psi_n^0(\,\cdot\,;\Lambda) - (\mathscr{D} - \Lambda)^{-1}\gamma M_{\chi'}\psi_n^0(\,\cdot\,;\Lambda) \,. \tag{4.40}$$

Since $\psi_n^0(\,\cdot\,;\Lambda)$ is an eigenfunction of $\mathscr{D}_0$ with eigenvalue $\pi(\Lambda)$, one immediately deduces that $\psi_n(\,\cdot\,;\Lambda)$ is an eigenfunction of $\mathscr{D}$ with the same eigenvalue:

$$(\mathscr{D} - \pi(\Lambda))\psi_n(\,\cdot\,;\Lambda) = (\mathscr{D} - \pi(\Lambda))\chi\psi_n^0(\,\cdot\,;\Lambda) - [\mathscr{D}, \chi]\psi_n^0(\,\cdot\,;\Lambda) = 0 \,.$$

While the functions $x \mapsto \psi_n(x\,;\Lambda)$ grow at infinity in general, it has been shown that the direct integral of the lines spanned by these functions in the limit of $\Lambda \to E_+$, $|E| > a_n$, equals the absolutely continuous subspace of $\mathscr{D}$ (cf. [10, Sect. 4] for the precise statement).

Now recall the decomposition (4.28) of the standing waves $\psi_n^0(\,\cdot\,;\Lambda)$ into running waves of outgoing and incoming type, $\phi_n^0(\,\cdot\,;\Lambda)$ resp. $\phi_n^0(\,\cdot\,;\tau_n\Lambda)$. When this decomposition is inserted into the formula of Def. 4.7 the former disappear:

$$\psi_n(\,\cdot\,;\Lambda) = -(2\mathrm{i})^{-1}\left(M_\chi\phi_n^0(\cdot\,;\tau_n\Lambda) - (\mathscr{D} - \Lambda)^{-1}\gamma M_{\chi'}\phi_n^0(\cdot\,;\tau_n\Lambda)\right) \,. \tag{4.41}$$

Indeed, if $f \in L^2$ satisfies $\chi(\mathscr{D} - \lambda)f = 0$ for $\lambda \in \mathrm{FP}$, then we have

$$\chi f = (\mathscr{D} - \lambda)^{-1}(\mathscr{D} - \lambda)\chi f = (\mathscr{D} - \lambda)^{-1}[\mathscr{D}, \chi] f = (\mathscr{D} - \lambda)^{-1}\gamma\chi' f \,.$$

Since $\phi_n^0(\,\cdot\,;\lambda)$ is an L^2-eigenfunction of $\mathscr{D}_0$, the claim follows a priori for $\lambda \in \mathrm{FP}$ and, by analytic continuation, for all Λ.

Formula (4.41) expresses the solution in terms of the unperturbed incoming wave $\phi_n^0(\,\cdot\,;\tau_n\Lambda)$, and holds as an equality of sections on all of X. Note that on restricting to $M \subset X$ where $\chi = 0$, the formula simplifies to

$$\psi_n(x\,;\Lambda) = (2\mathrm{i})^{-1}\left((\mathscr{D} - \Lambda)^{-1}[\mathscr{D}, \chi]\phi_n^0\right)(x\,;\tau_n\Lambda) \qquad (x \in M) \,. \tag{4.42}$$

4.6. **Transfer coefficients and resolvent on cylinder components.** We now extend the scattering problem as follows: let $Y_\alpha \subset Y$ $(\alpha = 1, \ldots, N)$ be pairwise disjoint, closed, connected submanifolds such that

$$Y = \cup_{\alpha=1}^N Y_\alpha \,. \tag{4.43}$$

Points on the α^{th} cylinder $\mathbb{R}_+ \times Y_\alpha$ will be denoted by $x_\alpha := (r_\alpha\,, \xi_\alpha)$. All objects constructed previously for the cylinder $\mathbb{R}_+ \times Y$ now get an additional subscript α to indicate that they belong to the cylinder $\mathbb{R}_+ \times Y_\alpha$.

The tangential operator A (cf. (4.3)) decomposes as

$$A = \oplus_{\alpha=1}^{N} A_\alpha \,, \tag{4.44}$$

and the eigenvalues resp. eigenmodes of A_α will now be denoted by $a_{\alpha n}$ resp. $\varphi_{\alpha n}$. By Σ we still denote the Riemann surface of the functions $\sqrt{\lambda^2 - a^2}$ where a runs through the positive eigenvalues of A. We put $k_{\alpha n}(\Lambda) = \sqrt{\Lambda^2 - a_{\alpha n}^2}$ for $\Lambda \in \Sigma$.

The eigenmode $\varphi_{\alpha n}$ is supported, of course, on Y_α, so that the running and standing free waves $\phi^0_{\alpha n}$ and $\psi^0_{\alpha n}$ are supported on $\mathbb{R}_+ \times Y_\alpha$. Note that for $\lambda \in \mathrm{FP}$ the resolvent $(\mathscr{D} - \lambda)^{-1}$ maps L^2-sections to L^2-sections. Hence the Lippmann–Schwinger equation shows that the scattering state $\psi_{\alpha n}$ of Def. 4.7 has the following properties:

(1) If $\lambda \in \mathrm{FP}$ the restriction of $\psi_{\alpha n}(\cdot\,;\lambda)$ to the cylinder $\mathbb{R}_+ \times Y_\beta$, $\beta \neq \alpha$, is square-integrable.
(2) On the cylinder $\mathbb{R}_+ \times Y_\alpha$ the difference $\psi_{\alpha n}(\cdot\,;\lambda) - \psi^0_{\alpha n}(\cdot\,;\lambda)$, $\lambda \in \mathrm{FP}$, is square-integrable.

The square-integrable part of $\psi_{\alpha n}(\cdot\,;\lambda)$ can be expanded in terms of the functions $\phi^0_{\alpha n}(\cdot\,;\lambda)$. Consequently (see [6, Sec. 5,7]) we have

Proposition 4.8. *There exist such meromorphic functions $T^{\alpha,\beta}_{m,n}(\Lambda)$ on Σ that on $\mathbb{R}_+ \times Y_\alpha$ we have expansions*

$$\psi_{\beta n}(x_\alpha\,;\Lambda) \approx -\frac{1}{2\mathrm{i}} \begin{cases} \phi^0_{\beta n}(x_\beta\,;\tau_{\beta n}\Lambda) + \sum\limits_m \phi^0_{\beta m}(x_\beta\,;\Lambda)\, T^{\beta,\beta}_{m,n}(\Lambda)\,, & \alpha = \beta\,, \\ \sum\limits_m \phi^0_{\alpha m}(x_\alpha\,;\Lambda)\, T^{\alpha,\beta}_{m,n}(\Lambda)\,, & \alpha \neq \beta\,, \end{cases}$$

which are to be understood as follows: for $\Lambda \in \mathrm{FP}$ (the physical sheet) the sum $\sum_m$ converges in the L^2-sense and the expansion is an equality; the individual terms are then extended meromorphically to Σ.

We refer to the functions $T^{\alpha,\beta}_{m,n}(\Lambda)$ as transfer coefficients (not to be confused with matrix entries of the so-called transfer matrix). They are closely related to scattering matrix elements, as will be explained in the last section of this paper.

The transfer coefficients $T^{\alpha,\beta}_{m,n}(\Lambda)$ can be calculated from the asymptotic form of the functions $\psi_{\beta n}(x_\alpha\,;\Lambda)$ by projection onto the outgoing running waves, as follows. Let $\Lambda_1, \Lambda_2 \in \Sigma$ with $\overline{\pi(\Lambda_1)} = \pi(\Lambda_2)$, and for any $r_\alpha > 0$ consider the integral

$$J^{\alpha,\beta}_{m,n}(\Lambda_1, \Lambda_2) := \int_{Y_\alpha} h\left(\phi^0_{\alpha m}(r_\alpha, \xi_\alpha\,;\Lambda_1), \mathrm{i}\gamma_\alpha \psi_{\beta n}(r_\alpha, \xi_\alpha\,;\Lambda_2)\right) d\xi_\alpha\,. \tag{4.45}$$

By the reasoning of the proof of Prop. 4.3, this indeed is independent of $r_\alpha > 0$.

Proposition 4.9. *For $\Lambda_1, \Lambda_2 \in \Sigma$ with $\overline{\pi(\Lambda_1)} = \pi(\Lambda_2) \neq 0$, define $J^{\alpha,\beta}_{m,n}(\Lambda_1, \Lambda_2)$ by Eq.* (4.45)*. Then, if $\alpha \neq \beta$,*

$$J^{\alpha,\beta}_{m,n}(\Lambda_1, \Lambda_2) = (-2\mathrm{i})^{-1} I^\alpha_{m,m}(0\,;\Lambda_1, \Lambda_2)\, T^{\alpha,\beta}_{m,n}(\Lambda_2)\,. \tag{4.46}$$

Proof. Let $\Lambda_2 \in \mathrm{FP}$, in which case the expansion of Prop. 4.8 for $\psi_{\beta n}(\,\cdot\,;\Lambda_2)$ is L^2-convergent. Inserting it, for $\alpha \neq \beta$, into the right-hand side of (4.45) one obtains

$$-2\mathrm{i} J^{\alpha,\beta}_{m,n}(\Lambda_1, \Lambda_2) = \sum\nolimits_k I^\alpha_{m,k}(r_\alpha\,;\Lambda_1, \Lambda_2) T^{\alpha,\beta}_{k,n}(\Lambda_2) = I^\alpha_{m,m}(0\,;\Lambda_1, \Lambda_2) T^{\alpha,\beta}_{m,n}(\Lambda_2)\,,$$

where Prop. 4.3 was used. The claim now follows by analytic continuation in Λ_2. □

In the case of $\alpha = \beta$ there may be another term due to the incoming wave in the expansion of Prop. 4.8. This term is absent in the following situation.

Proposition 4.10. *For any pair α, β and $\Lambda \in \Sigma$ we have that*

$$T^{\alpha,\beta}_{m,n}(\Lambda) = -\frac{2\mathrm{i}\pi(\Lambda)}{k_{\alpha m}(\Lambda)} J^{\alpha,\beta}_{m,n}(\tau_{\alpha m}\overline{\Lambda}, \Lambda)\,. \tag{4.47}$$

Proof. The restriction $\alpha \neq \beta$ in Prop. 4.9 becomes void on setting $\Lambda_2 = \Lambda$ and $\Lambda_1 = \tau_{\alpha m}\overline{\Lambda}$. Indeed, the extra term from the incoming wave in $\psi_{\beta n}(\,\cdot\,;\Lambda)$ for $\alpha = \beta$ and $m = n$ is then proportional to $I^{\alpha}_{n,n}(0\,;\tau_{\alpha n}\overline{\Lambda}\,,\tau_{\alpha n}\Lambda)$, which vanishes by Prop. 4.3. Thus if $\tau_{\alpha m}\overline{\Lambda_1} = \Lambda_2$ formula (4.46) holds for all $\alpha\,,\beta$. By using Eq. (4.35) for $I^{\alpha}_{m,m}(0\,;\tau_{\alpha m}\overline{\Lambda}\,,\Lambda)$ we then arrive at the proposed statement. □

Next we discuss the asymptotic expansion of the resolvent kernel of $\mathscr{D}$ on the cylinders. Notice that if we take $\lambda \in \mathrm{FP}$ and fix some point $x \in X$ outside of the cylinder $\mathbb{R}_+ \times Y_\alpha$, then

$$\mathbb{R}_+ \times Y_\alpha \ni x_\alpha \mapsto (\mathscr{D} - \lambda)^{-1}\,(x, x_\alpha)$$

is a square-integrable eigensection of $\mathscr{D}$. This eigensection maps into the bundle $E_x \otimes E^*$. Hence it has an expansion in terms of the running waves $\phi^0_{\alpha n}(x_\alpha\,;\overline{\lambda})$ $(n \in \mathbb{N})$ with coefficients in E_x :

Proposition 4.11. *For $x \in X \setminus (\mathbb{R}_+ \times Y_\alpha)$ and $\lambda \in \mathrm{FP}$ we have two L^2-convergent expansions on the cylinder $\mathbb{R}_+ \times Y_\alpha$:*

$$(\mathscr{D} - \lambda)^{-1}(x, x_\alpha) = \sum_n \frac{2\pi(\lambda)}{k_{\alpha n}(\lambda)}\,\psi_{\alpha n}(x\,;\lambda) \otimes h\left(\phi^0_{\alpha n}(x_\alpha\,;\overline{\lambda}),\,\cdot\,\right)\,, \tag{4.48}$$

and

$$(\mathscr{D} - \lambda)^{-1}(x_\alpha, x) = \sum_n \frac{2\pi(\lambda)}{k_{\alpha n}(\lambda)}\,\phi^0_n(x_\alpha\,;\lambda) \otimes h\left(\psi_n(x\,;\overline{\lambda}),\cdot\,\right)\,. \tag{4.49}$$

Proof. On the cylinder $\mathbb{R}_+ \times Y_\alpha$ we have an L^2-convergent expansion

$$(\mathscr{D} - \lambda)^{-1}(x, x_\alpha) =: 2\mathrm{i}\sum_n Q_n(x\,;\lambda) \otimes h\left(\phi^0_{\alpha n}(x_\alpha\,;\overline{\lambda}),\,\cdot\,\right) \qquad (\lambda \in \mathrm{FP}), \tag{4.50}$$

with a priori unknown coefficients $Q_n(x\,;\lambda) \in E_x$. Substituting this expansion into the Lippmann-Schwinger formula (4.42) we obtain

$$\begin{aligned}
&\psi_{\alpha n}(x\,;\lambda) = \\
&= \sum_m Q_m(x\,;\lambda) \int\limits_{\mathbb{R}_+ \times Y_\alpha} h\left(\phi^0_{\alpha m}(x_\alpha\,;\overline{\lambda}), \gamma_\alpha \chi'(x_\alpha)\phi^0_{\alpha n}(x_\alpha\,;\tau_{\alpha n}\lambda)\right) \mathrm{dvol}(x_\alpha) \\
&= -\mathrm{i}\sum_m Q_m(x\,;\lambda) \lim_{R\to\infty} \int\limits_{\{R\}\times Y_\alpha} h\left(\phi^0_{\alpha m}(R\,,\xi_\alpha\,;\overline{\lambda}), \mathrm{i}\gamma_\alpha \phi^0_{\alpha n}(R\,,\xi_\alpha\,;\tau_{\alpha n}\lambda)\right) d\xi_\alpha\,.
\end{aligned}$$

The second step follows after partially integrating w.r.t. the longitudinal coordinate r_α and once again using Prop. 3.5 (cf. also (4.31)). The lower boundary term vanishes because χ is zero at $r_\alpha = 0$. What we have obtained is the familiar integral (4.31). By using Prop. 4.3 we find

$$\psi_{\alpha n}(x\,;\lambda) = -\mathrm{i}\sum_m Q_m(x\,;\lambda) \lim_{R\to\infty} I^{\alpha}_{m,n}(R\,;\overline{\lambda}\,,\tau_{\alpha n}\lambda) = \mathrm{i}Q_n(x\,;\lambda)\,k_{\alpha n}(\lambda)/\pi(\lambda)\,.$$

Thus the coefficients in the expansion (4.50) are given by

$$\mathrm{i}Q_n(x\,;\lambda) = \frac{\pi(\lambda)}{k_{\alpha n}(\lambda)}\,\psi_{\alpha n}(x\,;\lambda)\,,$$

and (4.48) is proved.

Since $\mathscr{D}$ is self-adjoint the resolvent kernel has the symmetry property

$$(\mathscr{D} - \lambda)^{-1}(x, y) = \left((\mathscr{D} - \overline{\lambda})^{-1}\right)^{\dagger}(y, x)\,, \tag{4.51}$$

for arbitrary $x, y \in X$. Using it, (4.49) follows immediately from (4.48) by taking adjoints. □

4.7. **Transport conductance and the scattering matrix.** We now turn to the conductivity bi-vector field introduced in Sect. 3.4, and compute the double flux integral (2.17). Thus for $\xi \in T_x^* X$ and $\eta \in T_y^* X$ let

$$\langle g_{\Lambda_1,\, \Lambda_2}(x,y), (\xi,\eta)\rangle := \operatorname{tr}\left(\mathrm{ic}(\xi)\, (\mathscr{D}-\Lambda_1)^{-1}(x,y)\, \mathrm{ic}(\eta)\, (\mathscr{D}-\Lambda_2)^{-1}(y,x)\right) \ ,$$

which is the contribution to the conductivity bi-vector field $\sigma_{\lambda,\lambda'}$ from the first term on the right-hand side of the formula of Definition 3.10.

Let then Y_α, Y_β be two different boundary faces, $\alpha \neq \beta$. Our goal is to calculate the double flux integral of the bi-vector field $g_{\Lambda_1,\, \Lambda_2}$ through Y_α and Y_β :

$$F_{\beta,\, \alpha}(\Lambda_1,\, \Lambda_2) := -\int_{Y_\beta}\int_{Y_\alpha} \langle g_{\Lambda_1,\, \Lambda_2}(x_\beta, x_\alpha), (dr_\beta, dr_\alpha)\rangle d\xi_\alpha d\xi_\beta \tag{4.52}$$

for $\pi(\Lambda_1) = \pi(\Lambda_2)$, and in particular for $\Lambda_1 = E_+$, $\Lambda_2 = E_-$, $E \in \mathbb{R} \setminus (S \cup -S)$. This will already yield the transport conductance, $(G_{\mathrm{tr}})_{\alpha\beta}(E) = F_{\alpha,\, \beta}(E_+, E_-)$, since all terms beyond the first one in the formula of Definition 3.10 give zero due to the orthogonality relations of Proposition 4.4. Before stating the result, we remind the reader that for Λ_1 , $\Lambda_2 \in \Sigma$ with $\pi(\Lambda_1) = \pi(\Lambda_2)$ and $a \in S$ we have

$$\sqrt{\Lambda_1^2 - a^2} = \pm\sqrt{\Lambda_2^2 - a^2}\, . \tag{4.53}$$

Also, by the definition of the Riemann surface Σ we have $\operatorname{Im}\sqrt{\Lambda_j^2 - a^2} > 0$ for a large enough. Therefore we obtain:

Lemma 4.12. *Let Λ_1 , $\Lambda_2 \in \Sigma$ with $\pi(\Lambda_1) = \pi(\Lambda_2)$. Then $\sqrt{\Lambda_1^2 - a^2} = \sqrt{\Lambda_2^2 - a^2}$ for all but finitely many $a \in S$.*

Theorem 4.13. *Let $\alpha \neq \beta$. Furthermore, let Λ_1 , $\Lambda_2 \in \Sigma$ with $\pi(\Lambda_1) = \pi(\Lambda_2)$. Then the flux integral equals*

$$F_{\beta,\alpha}(\Lambda_1, \Lambda_2) = {\sum_{m,n}}' \frac{k_{\beta n}(\Lambda_1)}{k_{\alpha m}(\Lambda_1)} \overline{T^{\beta,\alpha}_{n,m}(\overline{\Lambda_2})} T^{\beta,\alpha}_{n,m}(\Lambda_1)\ , \tag{4.54}$$

where $\sum'$ means summation over those m, n for which $k_{\alpha m}(\Lambda_1) = -k_{\alpha m}(\Lambda_2)$ and $k_{\beta n}(\Lambda_2) = -k_{\beta n}(\Lambda_1)$.

Remark 4.14. We explicitly point to the special case $\Lambda_1 = E_+$, $\Lambda_2 = E_-$, where $\pi(\Lambda_1) = \pi(\Lambda_2) = E$. In that case Theorem 4.13 yields

$$F_{\beta,\alpha}(E_+, E_-) = \sum_{a_{\alpha m},\, a_{\beta n} < |E|} \frac{\sqrt{E^2 - a_{\beta n}^2}}{\sqrt{E^2 - a_{\alpha m}^2}} \left|T^{\beta,\alpha}_{n,m}(E_+)\right|^2 \ .$$

The square-root factors arise from our unconventional choice of normalization for the scattering waves. Absorbing them into the transfer coefficients, we obtain the *Landauer-Büttiker formula*

$$(G_{\mathrm{tr}})_{\beta\alpha}(E) = F_{\beta,\alpha}(E_+, E_-) = \sum_{a_{\alpha m},\, a_{\beta n} < |E|} \left|S^{\beta,\alpha}_{n,m}(E_+)\right|^2 \ , \tag{4.55}$$

where $S^{\beta,\alpha}_{n,m}$ now are true scattering matrix elements, defined with respect to a basis of scattering waves that satisfy the unit flux normalization rule.

The proof of Theorem 4.13 will basically follow from the expansions (4.48), (4.49) and that of Proposition 4.8. There are, however, some technical difficulties to overcome, which stem from the fact that the expansions are L^2-convergent only on the physical sheet FP. In fact, for the pair (Λ_1, Λ_2) in Theorem (4.13) at least one of Λ_1 or Λ_2 will not be in FP, except in the trivial case $\Lambda_1 = \Lambda_2$.

Proposition 4.15. *Let $x \in X \setminus (\mathbb{R}_+ \times Y_\alpha)$, $\eta \in T_x^* M$. Furthermore, consider Λ_1, $\Lambda_2 \in \Sigma$ with $\pi(\Lambda_1) = \pi(\Lambda_2)$. Then*

$$\begin{aligned} F_\alpha(x, \eta\,; \Lambda_1, \Lambda_2) &:= \int_{Y_\alpha} \langle g_{\Lambda_1,\Lambda_2}(x, x_\alpha), (\eta, dr_\alpha)\rangle \, d\xi_\alpha \\ &= {\sum_m}' \frac{4\pi(\Lambda_1)}{k_{\alpha m}(\Lambda_1)} \, h\big(\psi_{\alpha m}(x; \overline{\Lambda_2}), \mathrm{i}c(\eta)\psi_{\alpha m}(x; \Lambda_1)\big) \; . \end{aligned} \tag{4.56}$$

Here, similarly as in Theorem 4.13 the primed sum ${\sum_m}'$ denotes summation over those m for which $k_{\alpha m}(\Lambda_1) = -k_{\alpha m}(\Lambda_2)$.

Remark 4.16. Note that by the very definition of the Riemann surface Σ the condition $k_{\alpha m}(\Lambda_1) = -k_{\alpha m}(\Lambda_2)$ cannot be satisfied for more than finitely many m. Thus $\sum'$ in Proposition 4.15 is in fact a finite sum.

Proof. Assume for the moment that $\Lambda_2 \in \mathrm{FP}$. Then Prop. 4.11, Eq. (4.49), yields

$$\begin{aligned} &F_\alpha(x, \eta\,; \Lambda_1, \Lambda_2) = \sum_m \frac{2\pi(\Lambda_2)}{k_{\alpha m}(\Lambda_2)} \times \\ &\int_{Y_\alpha} h\big(\psi_{\alpha m}(x; \overline{\Lambda_2})\,,\, \mathrm{i}c(\eta)(\mathscr{D} - \Lambda_1)^{-1}(x, x_\alpha)\; \mathrm{i}\gamma_\alpha \phi^0_{\alpha m}(r_\alpha, \xi_\alpha; \Lambda_2)\big) d\xi_\alpha \; . \end{aligned} \tag{4.57}$$

The integrals under the sum are certainly analytic in Λ_1 and Λ_2. Now we first evaluate the integral under the sum for the case of $\Lambda_1 \in \mathrm{FP}$. For that, we may insert the asymptotic expansion (4.48) for the resolvent to find

$$\begin{aligned} &\int_{Y_\alpha} h\big(\psi_{\alpha m}(x; \overline{\Lambda_2})\,,\, \mathrm{i}c(\eta)(\mathscr{D} - \Lambda_1)^{-1}(x, x_\alpha)\, \mathrm{i}\gamma_\alpha \phi^0_{\alpha m}(r_\alpha, \xi_\alpha; \Lambda_2)\big) d\xi_\alpha \\ &= \sum_n \frac{2\pi(\Lambda_1)}{k_{\alpha n}(\Lambda_1)} I^\alpha_{n,m}(r_\alpha; \overline{\Lambda}_1, \Lambda_2)\, h\big(\psi_{\alpha m}(x; \overline{\Lambda}_2),\, \mathrm{i}c(\eta)\psi_{\alpha n}(x; \Lambda_1)\big) \\ &= \frac{2\pi(\Lambda_1)}{k_{\alpha m}(\Lambda_1)} I^\alpha_{m,m}(0\,; \overline{\Lambda_1}, \Lambda_2)\, h\big(\psi_{\alpha m}(x; \overline{\Lambda}_2), \mathrm{i}c(\eta)\psi_{\alpha m}(x; \Lambda_1)\big) \; . \end{aligned} \tag{4.58}$$

From Proposition 4.3 we know that the integral $I^\alpha_{m,m}(0\,; \Lambda_1, \Lambda_2)$ vanishes unless $k_{\alpha m}(\Lambda_2) = \overline{k_{\alpha m}(\overline{\Lambda_1})} = -k_{\alpha m}(\Lambda_1)$. Thus it follows that

$$F_\alpha(x, \eta\,; \Lambda_1, \Lambda_2) = {\sum_m}' \frac{4\pi(\Lambda_1)}{k_{\alpha m}(\Lambda_1)} \, h\big(\psi_{\alpha m}(x; \overline{\Lambda_2}), \mathrm{i}c(\eta)\psi_{\alpha m}(x; \Lambda_1)\big) \; ,$$

with the sum being restricted by $k_{\alpha m}(\Lambda_2) = -k_{\alpha m}(\Lambda_1)$. By analytic continuation we now see that for all Λ_1, $\Lambda_2 \in \Sigma$ with $\pi(\Lambda_1) = \pi(\Lambda_2)$ the integral under the sum on the right-hand side of (4.57) is given by (4.58). This proves the proposition. □

Proof of Theorem 4.13. It remains to integrate the finite sum on the right-hand side of (4.56) over $x \in Y_\beta$. Hence we need to calculate

$$\int_{Y_\beta} h\big(\psi_{\alpha m}(r_\beta, \xi_\beta; \overline{\Lambda_2}), \mathrm{i}\gamma_\beta \psi_{\alpha m}(r_\beta, \xi_\beta; \Lambda_1)\big) d\xi_\beta. \tag{4.59}$$

Repeating the line of argument in the proof of Proposition 4.15 we may insert the asymptotic expansion of Proposition 4.8 for $\psi_{\alpha m}$ on the cylinder $\mathbb{R}_+ \times Y_\beta$. Together with Proposition 4.9 we obtain

$$\begin{aligned} \ldots &= \frac{1}{2\mathrm{i}} \sum_n \overline{T^{\beta,\alpha}_{n,m}(\overline{\Lambda_2})} \int_{Y_\beta} h\big(\phi^0_{\beta n}(r_\beta, \xi_\beta; \overline{\Lambda_2}), \mathrm{i}\gamma_\beta \psi_{\alpha m}(r_\beta, \xi_\beta; \Lambda_1)\big) d\xi_\beta \\ &= \frac{1}{4} \sum_n \overline{T^{\beta,\alpha}_{n,m}(\overline{\Lambda_2})}\, T^{\beta,\alpha}_{n,m}(\Lambda_1) I^\beta_{n,n}(0\,; \overline{\Lambda_2}, \Lambda_1). \end{aligned} \tag{4.60}$$

Finally, we insert this result into (4.56) integrated over Y_β. Using once again Proposition 4.3 we then obtain

$$F_{\beta,\alpha}(\Lambda_1, \Lambda_2) = \sum_{m,n} \frac{k_{\beta n}(\Lambda_1)}{k_{\alpha m}(\Lambda_1)} \overline{T^{\beta,\alpha}_{n,m}(\overline{\Lambda_2})}\, T^{\beta,\alpha}_{n,m}(\Lambda_1) ,$$

which is the desired result. □

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