Weierstraß-Institut

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The Cayley transform applied to
non-interacting quantum transport

Dedicated to the memory of Markus Büttiker (1950-2013)

Horia D. Cornean [1], Hagen Neidhardt [2], Lukas Wilhelm[2], Valentin A. Zagrebnov [3]

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[1] Department of Mathematical Sciences
    Aalborg University
    Fredrik Bajers Vej 7
    9220 Aalborg
    Denmark
    E-Mail: cornean@math.aau.dk

[2] Weierstrass Institute
    Mohrenstr. 39
    10117 Berlin
    Germany
    E-mail: hagen.neidhardt@wias-berlin.de
              lukas.c.wilhelm@googlemail.com

[3] Département de Mathématiques
    Université d'Aix-Marseille and
    Laboratoire d'Analyse, Topologie, Probabilités (UMR 7353)
    Centre de Mathématique et Informatique-AMU
    Technopôle Château-Gombert
    39, rue F. Joliot Curie, 13453 Marseille Cedex 13
    France
    E-Mail: Valentin.Zagrebnov@latp.univ-mrs.fr

Abstract

We extend the Landauer-Büttiker formalism in order to accommodate both unitary and self-adjoint operators which are not bounded from below. We also prove that the pure point and singular continuous subspaces of the decoupled Hamiltonian do not contribute to the steady current. One of the physical applications is a stationary charge current formula for a system with four pseudo-relativistic semi-infinite leads and with an inner sample which is described by a Schrödinger operator defined on a bounded interval with dissipative boundary conditions. Another application is a current formula for electrons described by a one dimensional Dirac operator; here the system consists of two semi-infinite leads coupled through a point interaction at zero.

1 Introduction

Considering a problem in quantum statistical mechanics and solid state physics Lifshits [21] found that there is a unique real-valued function $\xi(\cdot) \in L^1(\mathbb{R}, d\lambda)$ such that the formula

$$\text{tr}(\Phi(H_0 + V) - \Phi(H_0)) = \int_{\mathbb{R}} \xi(\lambda)\Phi'(\lambda)d\lambda \tag{1}$$

is valid for a suitable class of functions $\Phi(\cdot)$ guaranteeing that $\Phi(H_0 + V) - \Phi(H_0)$ is a trace class operator. Here H_0 is a self-adjoint operator and V is a finite dimensional self-adjoint operator. Formula (1) and function $\xi(\cdot)$ are known in the literature as trace formula and spectral shift function, respectively.

Inspired by the work of Lifshits the trace formula was carefully investigated and generalized by Krein, cf. [17]. In a first step Krein has shown that Lifshits' result remains true if V is a self-adjoint trace class operator. Later on he generalized the result to pairs of self-adjoint operators $\mathcal{S} = \{H, H_0\}$ such that their resolvent difference is a trace class operator, cf. [18]. In the following we call those pairs trace class scattering systems. For trace class scattering systems there exists a real-valued function $\xi(\cdot) \in L^1(\mathbb{R}, \frac{d\lambda}{1+\lambda^2})$ called also the spectral shift function such that

$$\text{tr}\left(\Phi(H) - \Phi(H_0)\right) = \int_{\mathbb{R}} \xi(\lambda)\Phi'(\lambda)d\lambda \tag{2}$$

is valid for a suitable class of functions $\Phi(\cdot)$. In particular, the formula

$$\text{tr}\left((H-z)^{-1} - (H_0-z)^{-1}\right) = -\int_{\mathbb{R}} \frac{\xi(\lambda)}{(\lambda-z)^2}d\lambda, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

holds. In contrast to the spectral shift function defined by (2), the function $\xi(\cdot)$ defined by the last equation is now not unique and is only determined up to a real constant. To verify (2) Krein firstly proved a trace formula (1) for a pair $\mathcal{U} = \{U, U_0\}$ of unitary operators for which $U - U_0$ is a trace class operator, cf. [18]. Regarding U and U_0 as the Cayley transforms of H and H_0, respectively, Krein was able to establish (2).

If $\mathcal{S} = \{H, H_0\}$ is a trace class scattering system, then the wave operators

$$W_\pm(H, H_0) = s\text{-}\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}P^{ac}(H_0) \tag{3}$$

exist and are complete where $P^{ac}(H_0)$ is the projection onto the absolutely continuous subspace of H_0, see [3]. Let $\Pi(H_0^{ac})$ be a spectral representation of the absolutely continuous part H_0^{ac} of H_0, cf. Appendix C. Further, let $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ be the scattering matrix of the trace class scattering system $\mathcal{S}$ with respect to $\Pi(H_0^{ac})$. It turns out that there is a suitable chosen spectral shift function $\xi(\cdot)$ such that the so-called Birman-Krein formula

$$\det(S(\lambda)) = e^{-2\pi i\xi(\lambda)}.$$

holds for a.e. $\lambda \in \mathbb{R}$.

The quantity $T(\lambda) := \frac{1}{2\pi i}(I_{\mathfrak{h}(\lambda)} - S(\lambda))$, $\lambda \in \mathbb{R}$, is usually called the transition matrix, see (99), where $I_{\mathfrak{h}(\lambda)}$ denotes the fiber identity operator of the spectral representation $\Pi(H_0^{ac})$. In [23] Radulescu has shown that the transition matrix $\{T(\lambda)\}_{\lambda \in \mathbb{R}}$, the unperturbed operator H_0 and the perturbation V are related in a certain way. Indeed, if H_0 is bounded and V is trace class, then the formula

$$\mathrm{tr}(H_0^n W_+(H, H_0)V) = \int_{\mathbb{R}} \lambda^n \mathrm{tr}(T(\lambda)) d\lambda, \quad n = 0, 1, 2, \ldots,$$

is valid.

It turns out that the so-called Landauer-Büttiker formula is a further interesting example in this circle of relations linking scattering matrix, unperturbed operator and perturbation. From the physical point of view the Landauer-Büttiker formula gives the steady state charge current flowing trough a non-relativistic quantum device where the carriers are not self-interacting. It goes back to Landauer and Büttiker, cf. [20] and [6], and was initially derived by them using phenomenological arguments.

The physical setting is as follows: there is a small sample (the inner system) and at least two leads (for simplicity we only discuss the two lead case). At negative times, the leads are not coupled to the inner system. Each subsystem is in a state of thermal equilibrium. In particular, one assumes that in the leads the electrons are distributed according to the Fermi-Dirac distribution function. More precisely, if μ_j are the chemical potentials of the left and right leads, $j \in \{l, r\}$, then the energy distribution of lead j is $f_j(\lambda) = f_{FD}(\lambda - \mu_j)$ where:

$$f_{FD}(\lambda) = \frac{1}{1 + e^{\beta\lambda}}, \quad \lambda \in \mathbb{R}, \quad \beta > 0. \tag{4}$$

At time zero the leads are suddenly attached to the inner system and a current can flow from one lead to the other through the inner system. Landauer found by heuristic arguments (later refined by Büttiker) that the stationary current J of non-relativistic particles flowing through the system should be given by

$$J = \frac{\mathfrak{e}}{2\pi} \int_{\mathbb{R}} d\lambda \, |\sigma(\lambda)|^2(\lambda)\big(f_{FD}(\lambda - \mu_l) - f_{FD}(\lambda - \mu_r)\big) \tag{5}$$

where $\sigma(\lambda)$ is the so-called transmission coefficient between the leads, a cross-section arising from an appropriate scattering system, and $\mathfrak{e} > 0$ is the magnitude of the elementary charge. The current is directed from left to right if $J > 0$ and from right to left if $J < 0$. If $\mu_l > \mu_r$, then a straightforward computation shows that $J > 0$ which shows that the charge current is directed from the higher chemical potential to the lower one.

Several works have already been published in which this approach has been made rigorous, cf. [12, 1, 8, 22, 10, 9, 11]. One assumes that at negative times the system is described by (a decoupled) Hamiltonian H_0, while for positive times by (a coupled Hamiltonian) H. Until now it was always assumed that both Hamiltonians are bounded from below and that the difference between their resolvents raised to some integer power is trace class.

Since our paper only deals with operator theoretical aspects of quantum transport of quasi-free particles, some of the terminology used in quantum statistical mechanics will be strictly adapted to our limited needs. For us, a *density operator* is just any non-negative bounded operator. A density operator ρ is an *equilibrium state* of H_0 if it is a positive function of H_0. A density operator ρ is called a *steady state* of H_0 if ρ commutes with H_0. Note that with our definition, equilibrium states are steady states. If H_0 is a decoupled direct sum of several operators $\bigoplus h_j$, then a direct sum of individual equilibrium states $\bigoplus F_j(h_j)$ would provide us with a special class of steady states of H_0.

A *charge* is any bounded self-adjoint operator Q commuting with H_0. Following [1], the *steady current* $J_{\rho,Q}^{\mathcal{S}}$ related to a charge Q and a given initial steady state ρ of H_0 is proved to be given by

$$J_{\rho,Q}^{\mathcal{S}} := -i\mathrm{tr}(W_-(H, H_0)\rho W_-(H, H_0)^*[H, Q]) \tag{6}$$

provided the commutator $[H, Q]$ is well defined and H has no singular continuous spectrum. Following [1] the current is directed from the leads to the sample. If the commutator is not well defined, a regularization procedure was proposed in [1]. It consists in replacing the operators H and H_0 by bounded self-adjoint operators

$$H(\eta) := H(I + \eta H)^{-N} \quad \text{and} \quad H_0(\eta) := H_0(I + \eta H_0)^{-N}, \quad \eta > 0, \tag{7}$$

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for some large enough N, where for simplicity it is assumed that both operators are non-negative. Of course, $\mathcal{S}(\eta) = \{H(\eta), H_0(\eta)\}$ is also a trace class scattering system for which the current $J_{\rho,Q}^{\mathcal{S}(\eta)}$ is well defined. Finally, one sets

$$J_{\rho,Q}^{\mathcal{S}} := \lim_{\eta \to +0} J_{\rho,Q}^{\mathcal{S}(\eta)}. \tag{8}$$

We note that the absolutely continuous subspace $\mathfrak{H}^{ac}(H_0)$ reduces the initial steady state and the charge operator. Let

$$\rho_{ac} := \rho \upharpoonright \mathfrak{H}^{ac}(H_0) \quad \text{and} \quad Q_{ac} := Q \upharpoonright \mathfrak{H}^{ac}(H_0) \tag{9}$$

The restrictions ρ_{ac} and Q_{ac} commute with the absolutely continuous component H_0^{ac} of H_0.

Let $\Pi(H_0^{ac})$ be a spectral representation of the absolutely continuous part H_0^{ac} of H_0, cf. Appendix C. Since the components ρ_{ac} and Q_{ac} commute with H_0^{ac}, they are unitarily equivalent to multiplication operators induced by some density and charge fiber matrices $\{\rho_{ac}(\lambda)\}_{\lambda \in \mathbb{R}}$ and $\{Q_{ac}(\lambda)\}_{\lambda \in \mathbb{R}}$ in $\Pi(H_0^{ac})$, respectively. In [1] it was proved that the current $J_{\rho,Q}^{\mathcal{S}}$ admits the representation

$$J_{\rho,Q}^{\mathcal{S}} = \frac{1}{2\pi} \int_{\mathbb{R}} d\lambda \, \text{tr} \left\{ \rho_{ac}(\lambda) \left(Q_{ac}(\lambda) - S(\lambda)^* Q_{ac}(\lambda) S(\lambda) \right) \right\}. \tag{10}$$

The formula (10) can be called the abstract Landauer-Büttiker formula. The formula (10) is not identical with the traditional Landauer and Büttiker formula (5). However, it was shown in [1] that formula (5) follows from (10).

The aim of the present paper is to extend the representation (10) to situations where the operators H and H_0 might not be bounded from below. Using the intertwining property of the wave operator and the trace cyclicity, one can rewrite the current $J_{\rho,Q}^{\mathcal{S}}$ in the following form:

$$J_{\rho,Q}^{\mathcal{S}} := -i\text{tr}(W_-(H, H_0)(I + H_0^2)\rho W_-(H, H_0)^*(H - i)^{-1}[H, Q](H + i)^{-1}). \tag{11}$$

It turns out that (11) can be expressed in a different form using the Cayley transforms

$$U = (i - H)(i + H)^{-1} = e^{2i \arctan(H)} \quad \text{and} \quad U_0 = (i - H_0)(i + H_0)^{-1} = e^{2i \arctan(H_0)}$$

of H and H_0, respectively. Under the condition that $V := U - U_0 = 2i((i + H)^{-1} - (i + H_0)^{-1})$ is a trace class operator we have

$$\Omega_\pm(U, U_0) := \text{s-} \lim_{n \to \pm\infty} U^n U_0^{-n} P^{ac}(U_0) =$$
$$W_\pm(2\arctan(H), 2\arctan(H_0)) = W_\pm(H, H_0),$$

where in the last equality we used the invariance principle of wave operators. Moreover, using the identity

$$-\frac{i}{2} U^*[U - U_0, Q] = (H - i)^{-1}[H, Q](H + i)^{-1}$$

the current can be rewritten as

$$J_{\tilde{\rho},Q}^{\mathcal{U}} := -\frac{1}{2} \text{tr}(\Omega_-(U, U_0)\tilde{\rho} U_0^* \Omega_-(U, U_0)^*[V, Q]), \quad V := U - U_0, \quad \tilde{\rho} := (1 + H_0^2)\rho, \tag{12}$$

where everything only depends on the unitary scattering system $\mathcal{U} := \{U, U_0\}$. Following Birman and Krein [18, 3] we start with the abstract unitary scattering system $\mathcal{U} := \{U, U_0\}$ where $V = U - U_0$ is trace class operator, $\tilde{\rho}$ is an initial steady state and Q a charge both commuting with U_0. Their restrictions to the absolutely continuous subspace of U_0 are denoted by $\tilde{\rho}_{ac}$ and Q_{ac}, respectively. Using a spectral representation of U_0, we denote by $\{\tilde{S}(\zeta)\}_{\zeta \in \mathbb{T}}$, $\{\tilde{\rho}_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$ and $\{\tilde{Q}_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$ the scattering, density and charge fiber matrices of $S = \Omega_+(U, U_0)^* \Omega_-(U, U_0)$, $\tilde{\rho}_{ac}$ and Q_{ac}, respectively. We also suppose that the singular continuous spectrum $\sigma_{sc}(U)$ of U is empty (note that we allow $\sigma_{sc}(U_0) \neq \emptyset$). Then it will be proven in Theorem 3.7 and in Corollary 3.8 that the current in (12) admits the representation

$$J_{\tilde{\rho},Q}^{\mathcal{U}} = \frac{1}{4\pi} \int_{\mathbb{T}} \text{tr} \left\{ \tilde{\rho}_{ac}(\zeta) \left(\tilde{Q}_{ac}(\zeta) - \tilde{S}(\zeta)^* \tilde{Q}_{ac}(\zeta) \tilde{S}(\zeta) \right) \right\} d\nu(\zeta)$$
$$= \frac{1}{4\pi} \int_{\mathbb{T}} \text{tr} \left\{ \left(\tilde{\rho}_{ac}(\zeta) - \tilde{S}(\zeta) \tilde{\rho}_{ac}(\zeta) \tilde{S}(\zeta)^* \right) \tilde{Q}_{ac} \right\} d\nu(\zeta), \tag{13}$$

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where ν is the Haar measure with $\nu(\mathbb{T}) = 2\pi$.

More importantly, from the second formula above we see that if $\tilde{\rho}$ is an equilibrium state, i.e. some non-negative function $\tilde{f}(U_0)$, then it is a scalar multiplication with $\tilde{f}(\zeta)$ on each fiber $\tilde{\mathfrak{h}}(\lambda)$ and thus commutes with $\tilde{S}(\zeta)$ almost everywhere. This shows that the current is zero at equilibrium. Moreover, we can use this to renormalize the current by subtracting zero in the following way:

$$J_{\tilde{\rho},Q}^{\mathcal{U}} = \frac{1}{4\pi} \int_{\mathbb{T}} \mathrm{tr}\left\{ \left(\tilde{\rho}_{ac}(\zeta) - \tilde{f}(\zeta) I_{\tilde{\mathfrak{h}}(\zeta)} \right) \left(\tilde{Q}_{ac}(\zeta) - \tilde{S}(\zeta)^* \tilde{Q}_{ac}(\zeta)\tilde{S}(\zeta) \right) \right\} d\nu(\zeta). \tag{14}$$

Going back to the self-adjoint case via the Cayley transform, we have to change the torus with the real line by the transformation $\zeta = e^{2i\arctan(\lambda)}$. Hence, replacing $\tilde{\rho}(e^{2i\arctan(\lambda)})$ by $(1+\lambda^2)\rho(\lambda)$ and introducing $Q_{ac}(\lambda) := \tilde{Q}_{ac}(e^{2i\arctan(\lambda)})$ and $S(\lambda) := \tilde{S}(e^{2i\arctan(\lambda)})$ we obtain

$$J_{\rho,Q}^{\mathcal{S}} = \frac{1}{2\pi} \int_{\mathbb{R}} d\lambda \, \mathrm{tr}\left\{ \left(\rho_{ac}(\lambda) - f(\lambda) I_{\mathfrak{h}(\lambda)} \right) \left(Q_{ac}(\lambda) - S(\lambda)^* Q_{ac}(\lambda)S(\lambda) \right) \right\}. \tag{15}$$

This formula is very useful in the relativistic situation when $\rho_{ac}(\lambda)$ can loose its decay in λ at $-\infty$, as it happens with the Fermi-Dirac distribution. In that case we see that $\rho_{ac}(\lambda) - f_{FD}(\lambda) I_{\mathfrak{h}(\lambda)}$ still decays exponentially at $\pm\infty$ and the current will be finite.

Let us make the following remarks:

- Our main technical result is formula (13), proved in Theorem 3.7. It can be seen as an abstract Landauer-Büttiker formula for unitary scattering systems.

- Formula (10) is proved in Theorem 3.9, which is an extension of the result in [22], where $V := H - H_0 \in \mathfrak{L}_1(\mathfrak{H})$ was assumed.

- Another result related to Theorem 3.9 was proven in [1] where the current was defined through a regularization procedure. There the operators H and H_0 were replaced by $H(1 + \eta H)^{-N}$ and $H_0(1 + \eta H_0)^{-N}$, respectively, and the limit $\eta \to +0$ was taken outside the trace. Using our approach via the Cayley transforms one gets a definition of the current (see (12) or (11)) which avoids any regularization. Since the Cayley transform does not require H_0 and H to be bounded from below, it allows us to derive Landauer-Büttiker type formulas for self-adjoint dilations of maximal dissipative Schrödinger operators and Dirac operators with point interactions at zero, see Section 4.

- Our result is stronger than that one of [1]. At first glance it seems to be that the condition $(H + \theta)^{-N} - (H_0 + \theta)^{-N} \in \mathfrak{L}_1(\mathfrak{H})$ assumed in [1] for some $N \in \mathbb{N}$ and $\theta > 0$ is weaker than our condition $(i + H)^{-1} - (i + H_0)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$. Nevertheless, the result of [1] follows from Theorem 3.9. Indeed, let us assume for simplicity that $H \geq I$ and $H_0 \geq I$ as well as $\theta = 0$. A straightforward computation shows that the representation

$$J_{\rho,Q}^{\mathcal{S}} = -\frac{i}{N} \mathrm{tr}\left(W_-(H, H_0) \frac{I + H_0^{2N}}{H_0^{N-1}} \rho W_-(H, H_0)^*(H^N - i)^{-1}[H^N, Q](H^N + i)^{-1} \right) \tag{16}$$

is valid provide $(I + H_0^{N+1})\rho$ is a bounded operator. Therefore, considering the trace class scattering system $\widehat{\mathcal{S}} = \{H^N, H_0^N\}$, we find

$$J_{\rho,Q}^{\mathcal{S}} = \frac{1}{N} J_{\widehat{\rho},Q}^{\widehat{\mathcal{S}}}, \qquad \widehat{\rho} := H_0^{-(N-1)}\rho,$$

where the invariance principle for wave operators was taken into account. Finally, applying Theorem 3.9 to $J_{\widehat{\rho},Q}^{\widehat{\mathcal{S}}}$ we get a Landauer-Büttiker formula for the scattering system $\widehat{\mathcal{S}} = \{H^N, H_0^N\}$ with respect to a spectral representation of $(H_0^N)^{ac}$. However, from the spectral representation of $(H_0^N)^{ac}$ one easily obtains a spectral representation of H_0^{ac} which immediately implies the result of [1].

- We can extend Theorem 3.9 to some situations where H and H_0 are not bounded from below and $(H + i)^{-1} - (H_0 + i)^{-1}$ is not trace class. Namely, if 0 belongs to the resolvent set of both H and H_0, and if there exists an odd integer N such that $H^{-N} - H_0^{-N}$ is trace class, then the invariance principle can still be applied and formula (1.16) (see also (1.12)) still makes sense. The general case remains open.

The paper is organized as follows. In Section 2 we review some well known results related to non equilibrium steady states and currents, and extend them to the case of non-semibounded self-adjoint operators H_0 and H. The main goal is to rigorously justify formula (12).

Section 3 is devoted to the proof of the abstract Landauer-Büttiker formula (13), at first for unitary operators, cf. Section 3.1, and then for self-adjoint operators, cf. Section 3.2.

In Section 4 we give several examples. Finally, in order to make the paper self-contained we have added Appendices A and B, C on spectral representations of unitary operators, and Appendix D on the scattering matrix of unitary operators.

Notation: By $\mathfrak{H}^{ac}(U)$ we denote the absolutely continuous subspace of a unitary operator U defined on $\mathfrak{H}$. The projection from $\mathfrak{H}$ onto $\mathfrak{h}^{ac}(U)$ is denoted by $P^{ac}(U)$. The corresponding absolutely continuous restriction of U is denoted by $U^{ac} := U \upharpoonright \mathfrak{H}^{ac}(U)$. The singular subspace of a unitary operator U is defined by $\mathfrak{H}^s(U) := \mathfrak{H} \ominus \mathfrak{H}^{ac}(U)$, the corresponding singular part by $U^s := U \upharpoonright \mathfrak{H}^s(U)$. A similar notation is used for self-adjoint operators.

Furthermore the real axis and the unit circle are denoted by $\mathbb{R}$, and $\mathbb{T}$ respectively. The open unit disc is denoted by $\mathbb{D} := \{\zeta \in \mathbb{C} : |\zeta| < 1\}$.

2 Steady states and currents

Let H_0 be a self-adjoint operator and let ρ be a steady state for H_0. Furthermore, let us assume that at $t < 0$ the system is described by the Hamiltonian H_0 and the steady state ρ. At $t = 0$ we switch on a coupling such that the system is now described by the Hamiltonian H. The state $\rho(t)$ evolves according to the quantum Liouville equation

$$i\frac{d\rho}{dt} = [H, \rho(t)], \quad t > 0, \quad \rho(0) = \rho,$$

which has the weak solution

$$\rho(t) = e^{-itH}\rho e^{itH}, \quad t \geq 0.$$

The operator $\rho(t)$ is a density operator, but not a steady state for H. However, one can produce a steady state by taking an ergodic limit as in [1]. It turns out that Theorem 3.2 of [1] remains true even if H and H_0 are not semibounded; for completeness we formulate and prove below the result.

Proposition 2.1. *Let H_0 be a self-adjoint operator and let ρ be a steady state of H_0. If H is another self-adjoint operator such that $(H + i)^{-1} - (H_0 + i)^{-1}$ is a trace class operator and $\sigma_{sc}(H) = \emptyset$, then the limit*

$$\rho_+ := \text{s-}\lim_{T \to \infty} \frac{1}{T} \int_0^T \rho(t)dt \tag{17}$$

exists and is given by

$$\rho_+ = W_-(H, H_0)\rho W_-(H, H_0)^* + \sum_{\lambda_k \in \sigma_p(H)} E_H(\{\lambda_k\})\rho E_H(\{\lambda_k\}) \tag{18}$$

where $E_H(\cdot)$ is the spectral measure of H and $\sigma_p(H)$ denotes the point spectrum of H, cf [1, Theorem 3.2]. Moreover, ρ_+ is a steady state of H.

Proof. We use the representation

$$\rho(t) = e^{-itH}e^{itH_0}\rho e^{-itH_0}e^{itH}P^{ac}(H) + e^{-itH}\rho e^{itH}P^p(H), \quad t \geq 0,$$

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where $P^p(H)$ denotes the projection onto the subspace spanned by the eigenvectors of H. Notice that $P^p(H) = P^s(H)$ where $P^s(H)$ is the projection onto the singular subspace of H. Since the resolvent difference is a trace class operator one gets

$$s\text{-}\lim_{T\to\infty} \frac{1}{T}\int_0^T e^{-itH}e^{itH_0}\rho e^{-itH_0}e^{itH}P^{ac}(H)dt = W_-(H,H_0)\rho W_-(H,H_0)^*.$$

Let $\lambda_k \in \sigma_p(H)$. We find

$$e^{-itH}\rho e^{itH}E_H(\{\lambda_k\}) = e^{-it(H-\lambda_k)}\rho E_H(\{\lambda_k\}), \quad t \geq 0.$$

If $f = (H - \lambda_k)g$, $g \in \mathrm{dom}(H)$, then

$$\frac{1}{T}\int_0^T e^{-it(H-\lambda_k)}f dt = \frac{e^{-iT(H-\lambda_k)} - I}{-iT}g$$

which yields

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T e^{-it(H-\lambda_k)}f dt = 0$$

Since $\mathrm{ran}(H - \lambda_k)$ is dense in $E_H(\mathbb{R} \setminus \{\lambda_k\})\mathfrak{H}$ we verify that

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T e^{-it(H-\lambda_k)}E_H(\mathbb{R} \setminus \{\lambda_k\})dt = 0$$

Finally, using the decomposition

$$e^{-itH}\rho e^{itH}E_H(\{\lambda_k\}) = e^{-it(H-\lambda_k)}E_H(\mathbb{R} \setminus \{\lambda_k\})\rho E_H(\{\lambda_k\})+$$
$$E_H(\{\lambda_k\})\rho E_H(\{\lambda_k\}), \quad t \geq 0,$$

which proves

$$s\text{-}\lim_{T\to\infty} \frac{1}{T}\int_0^T e^{-itH}\rho e^{itH}E_H(\{\lambda_k\})dt = E_H(\{\lambda_k\})\rho E_H(\{\lambda_k\}).$$

Using that we immediately prove (18). $\qquad\square$

Formally, the current $J^{\mathcal{S}}_{\rho,Q}$ is defined by

$$J^{\mathcal{S}}_{\rho,Q} = -\mathbb{E}_{\rho_+}(i[H,Q]) = -i\mathrm{tr}(\rho_+[H,Q]),$$

where $\mathbb{E}_{\rho_+}(\cdot)$ is the expectation value of an observable with respect to ρ_+. In general, the definition might be not correct because either the commutator $[H,Q]$ is not well-defined or the product $\rho_+ i[H,Q]$ is not a trace class operator. To avoid such difficulties we set

$$J^{\mathcal{S}}_{\rho,Q}(\delta) := -\mathbb{E}_{\rho_+}(iE_H(\delta)[H,Q]E_H(\delta)) = -i\mathrm{tr}(\rho_+ E_H(\delta)[H,Q]E_H(\delta)) \tag{19}$$

where δ is any bounded Borel set of $\mathbb{R}$. Furthermore, $E_H(\delta)[H,Q]E_H(\delta)$ is a well defined trace class operator for any bounded Borel set δ. Indeed, using the representation

$$E_H(\delta)[H,Q]E_H(\delta) = (H - i)E_H(\delta)KE_H(\delta)(H + i) \tag{20}$$

where

$$K := (H-i)^{-1}[H,Q](H+i)^{-1} = (H+i)(H-i)^{-1}[(H+i)^{-1},Q] \tag{21}$$
$$= (I + 2i(H-i)^{-1})[(H+i)^{-1} - (H_0+i)^{-1},Q]$$

is trace class. We get that $E_H(\delta)[H,Q]E_H(\delta)$ is a trace class operator for every bounded Borel set δ. We set

$$J^{\mathcal{S}}_{\rho,Q} := \lim_{\delta\to\mathbb{R}} J^{\mathcal{S}}_{\rho,Q}(\delta)$$

provided the limit exists. We show this now.

Proposition 2.2. *Let H_0 be a self-adjoint operator and let ρ be a steady state for H_0 and let H be a self-adjoint operator. Further, let Q be a charge for H_0. If the resolvent difference of H and H_0 is a trace class operator, $\sigma_{sc}(H) = \emptyset$ and $(I + H_0^2)\rho$ is a bounded operator, then the current $J_{\rho,Q}^{\mathcal{S}}$ is well-defined and admits the representation* (11).

Proof. Inserting (20) into (19) we get

$$J_{\rho,Q}^{\mathcal{S}}(\delta) := i\mathrm{tr}(\rho_+(H-i)E_H(\delta)KE_H(\delta)(H+i))$$

where K is a trace class operator defined by (21). Using (18) we get

$$J_{\rho,Q}^{\mathcal{S}}(\delta) = -i\mathrm{tr}(W_-(H,H_0)\rho W_-(H,H_0)^*(H-i)E_H(\delta)KE_H(\delta)(H+i))$$

$$- i\sum\nolimits_{\lambda_k \in \sigma_p(H) \cap \delta} \mathrm{tr}(\rho E_H(\{\lambda_k\})(H-i)K(H+i)E_H(\{\lambda_k\})).$$

Since $E_H(\{\lambda_k\})KE_H(\{\lambda_k\}) = 0$ we find

$$J_{\rho,Q}^{\mathcal{S}}(\delta) = -i\mathrm{tr}(W_-(H,H_0)(H_0^2+I)\rho W_-(H,H_0)^*E_H(\delta)KE_H(\delta)),$$

where we have used that $(H_0^2 + I)\rho$ is a bounded operator. Then the limit in (2) exists and equals:

$$J_{\rho,Q}^{\mathcal{S}} = -i\mathrm{tr}(W_-(H,H_0)(H_0^2+I)\rho W_-(H,H_0)^*K).$$

Note that (21) coincides with (11). $\qquad\square$

3 Landauer-Büttiker formula for unitary scattering systems

3.1 Unitary operators

Let us recall that we consider two unitary operators U and U_0 such that $U - U_0$ is trace class, and a bounded self-adjoint operator Q commuting with U_0 is called a charge. Thus any charge Q is reduced by $\mathfrak{H}^{ac}(U_0)$ and $\mathfrak{H}^s(U_0)$. In other words, Q admits the decomposition $Q = Q_{ac} \oplus Q_s$ where $Q_{ac} := Q \upharpoonright \mathfrak{H}^{ac}(U_0)$ and $Q_s := Q \upharpoonright \mathfrak{H}^s(U_0)$. Notice that the restrictions Q_{ac} and Q_s might not be identical with the absolutely continuous and singular components Q^{ac} and Q^s, respectively.

Let $\Pi(U_0^{ac}) = \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$ be a spectral representation of U_0^{ac}, cf. Appendix A. Since Q_{ac} commutes with U_0^{ac} there is a measurable family $\{Q_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$ of bounded self-adjoint operators acting on $\mathfrak{h}(\zeta)$ such that

$$\nu - \sup_{\zeta \in \mathbb{T}} \|Q_{ac}(\zeta)\|_{\mathcal{B}(\mathfrak{h}(\zeta))} = \|Q_{ac}\|_{\mathcal{B}(\mathfrak{H})}$$

and $Q_{ac} = \Phi^{-1}M_{Q_{ac}}\Phi$ where $M_{Q_{ac}}$ is the multiplication operator induced by $\{Q_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$ in $L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$.

A non-negative bounded self-adjoint operator ρ commuting with U_0 is also called a density operator and admits the decomposition $\rho = \rho_{ac} \oplus \rho_s$. The part ρ_{ac} is unitarily equivalent to the multiplication operator $M_{\rho_{ac}}$ induced by a measurable family $\{\rho_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$ of non-negative bounded operators acting on $\mathfrak{h}(\zeta)$ and satisfying $\nu - \sup_{\zeta \in \mathbb{T}} \|\rho_{ac}(\zeta)\|_{\mathfrak{h}(\zeta)} = \|\rho_{ac}\|_{\mathfrak{H}}$ in $L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$.

Let $\mathcal{S} = \{U, U_0\}$ be an $\mathfrak{L}_1$-scattering system. Further, let Q be a charge and let ρ be a density operator. In this case we define the current J for $\mathcal{S}$ by

$$J := -\frac{1}{2}\mathrm{tr}(\Omega_-\rho U_0^*\Omega_-^*[V,Q]) \tag{22}$$

where $V = U - U_0$ is trace class and $[V,Q] = VQ - QV$. The main result of this section (see Proposition 3.5) will show that only the absolutely continuous restriction of Q contributes to the current:

$$J = J_{ac} := -\frac{1}{2}\mathrm{tr}(\Omega_-\rho U_0^*\Omega_-^*[V,Q_{ac}]). \tag{23}$$

Before that, we need a series of lemmata.

Lemma 3.1. *Let U_0 be a unitary operator on $\mathfrak{H}$ and let Q be a charge. Then $\mathfrak{H}$ admits an orthogonal decomposition*

$$\mathfrak{H} = \bigoplus_{k \in \mathbb{N}} \mathfrak{H}_k$$

reducing U_0 and Q such that $U_k := U_0 \upharpoonright \mathfrak{H}_k$, $k \in \mathbb{N}$, has a constant spectral multiplicity function and $Q_k := Q \upharpoonright \mathfrak{H}_k$ commutes with U_k, $k \in \mathbb{N}$.

Proof. Let $\Pi(U_0) = \{L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta)), M, \Psi\}$ be a spectral representation of U_0, cf Appendix A, and let $\mathrm{Mult}(\zeta) := \dim(\mathfrak{k}(\zeta))$ be the spectral multiplicity function of U_0. We set $\Delta_1 := \{\zeta \in \mathbb{T} : \mathrm{Mult}(\zeta) = \infty\}$ and $\Delta_k := \{\zeta \in \mathbb{T} : \mathrm{Mult}(\zeta) = k - 1\}$ if $k \geq 2$. Let $E_0(\cdot)$ be the spectral measure of U_0. We set $\mathfrak{H}_k := E_0(\Delta_k)\mathfrak{H}$. Obviously, each subspace $\mathfrak{H}_k$ reduces U_0 and Q. Moreover, the unitary operators U_k defined on $\mathfrak{H}_k$ are of constant spectral multiplicity. $\qquad\square$

Next we are going to show that Q can be approximated by a sequence of self-adjoint operators with pure point spectrum.

Lemma 3.2. *Let U_0 be a unitary operator on $\mathfrak{H}$ of constant spectral multiplicity and let Q be a charge. Then there is a sequence $\{Q_m\}_{m \in \mathbb{N}}$ of charges with pure point spectrum satisfying s-$\lim_{m \to \infty} Q_m = Q$ and $\|Q_m\|_{\mathfrak{H}} \leq \|Q\|_{\mathfrak{H}} + 1$.*

Proof. Since U_0 is of constant spectral multiplicity U_0 admits the spectral representation $\Pi(U_0) := \{L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}), M, \Psi\}$ where $\mathfrak{k}$ is independent from $\zeta \in \mathbb{T}$. If Q is a charge, then there is a measurable family $\{Q(\zeta)\}_{\zeta \in \mathbb{T}}$ of bounded self-adjoint operators satisfying $\mu - \sup_{\zeta \in \mathbb{T}}\|Q(\zeta)\|_{\mathfrak{k}} = \|Q\|_{\mathfrak{H}}$ such that Q is unitarily equivalent to the multiplication operator M_Q in $L^2(\mathbb{T}, \mu(\zeta), \mathfrak{k})$.

Since $\{Q(\zeta)\}_{\zeta \in \mathbb{T}}$ is a measurable family of self-adjoint operators there is a sequence $\{\widetilde{Q}_m(\zeta)\}_{\zeta \in \mathbb{T}}$ of simple functions such that

$$s\text{-}\lim_{m \to \infty} \widetilde{Q}_m(\zeta) = Q(\zeta) \tag{24}$$

for a.e. $\zeta \in \mathbb{T}$ with respect to μ. We recall that $\widetilde{Q}_m(\cdot)$ is simple if it admits the representation

$$\widetilde{Q}_m(\zeta) = \sum_l \chi_{\delta_{ml}}(\zeta)\widetilde{Q}_{ml}, \quad \zeta \in \mathbb{T}, \quad \widetilde{Q}_{ml} = \widetilde{Q}_{ml}^* \in \mathfrak{B}(\mathfrak{k}),$$

where $\{\delta_{ml}\}$ are disjoint Borel subsets of $\mathbb{T}$ satisfying $\bigcup_l \delta_{ml} = \mathbb{T}$ for each $m \in \mathbb{N}$ and $\sum_l$ is finite. Without loss of generality we can assume that the condition

$$\|\widetilde{Q}_m(\zeta)\|_{\mathfrak{k}} \leq \mu - \sup_{\eta \in \mathbb{T}}\|\widetilde{Q}_m(\eta)\|_{\mathfrak{k}}$$

is satisfied for each $m \in \mathbb{N}$.

By the v. Neumann theorem [15, Theorem X.2.1] for each self-adjoint operator $\widetilde{Q}_{ml}$ there is a self-adjoint Hilbert-Schmidt operator D_{ml} such that $\|D_{ml}\|_{\mathfrak{L}_2} \leq \frac{1}{m}$ and $Q_{ml} := \widetilde{Q}_{ml} + D_{ml}$ is pure point. Setting

$$Q_m(\zeta) = \sum_l \chi_{\delta_{ml}}(\zeta)Q_{ml}, \quad \zeta \in \mathbb{T}, \quad Q_{ml} = Q_{ml}^* \in \mathfrak{B}(\mathfrak{k}),$$

one easily verifies that

$$s\text{-}\lim_{m \to \infty} Q_m(\zeta) = Q(\zeta)$$

for a.e. $\zeta \in \mathbb{T}$ with respect to μ. We note that $s\text{-}\lim_{m \to \infty} M_{Q_m} = M_Q$. Moreover, the spectrum of M_{Q_m} is pure point for each $m \in \mathbb{N}$. Setting $Q_m := \Psi^{-1} M_{Q_m} \Psi$ we find that $s\text{-}\lim_{m \to \infty} Q_m = Q$. Moreover, each operator Q_m commutes with U_0. $\qquad\square$

Lemma 3.3. *Let U_0 be a purely singular unitary operator (i.e. the absolutely continuous component is absent) on the separable Hilbert space $\mathfrak{H}$. Then there is a sequence $\{U_n\}_{n \in \mathbb{N}}$ of unitary operators with pure point spectrum such that $U_0 - U_n \in \mathfrak{L}_1(\mathfrak{H})$, $n \in \mathbb{N}$, and $\lim_{n \to \infty} \|U_0 - U_n\|_{\mathfrak{L}_1} = 0$.*

Proof. Let us assume that $\ker(U_0 + I) = \{0\}$. We introduce the self-adjoint operator

$$H_0 = i(I - U_0)(I + U_0)^{-1}.$$

Since U_0 is singular the self-adjoint operator H_0 is also singular. By Lemma 2 of [7] for each $n \in \mathbb{N}$ there is a self-adjoint trace class operator D_n satisfying $\|D_n\|_{\mathfrak{L}_1} < \frac{1}{n}$ such that $\widetilde{H}_n := H_0 + D_n$ is pure point. Hence, the unitary operators

$$U_n := (i - \widetilde{H}_n)(i + \widetilde{H}_n)^{-1}, \quad n \in \mathbb{N},$$

have pure point spectrum. Since

$$U_0 - U_n = 2i(i + \widetilde{H}_n)^{-1}D_n(i + H_0)^{-1}, \quad n \in \mathbb{N},$$

we get

$$\|U_0 - U_n\|_{\mathfrak{L}_1} \le 2\|D_n\|_{\mathfrak{L}_1} < \frac{2}{n}, \quad n \in \mathbb{N},$$

which yields $s\text{-}\lim_{n\to\infty} \|U_0 - U_n\|_{\mathfrak{L}_1} = 0$.

If the condition $\ker(I + U_0) = 0$ is not satisfied, then the unitary operator admits the decomposition $U_0 = U_0' \oplus U_0''$ where $U_0' = U_0 \upharpoonright \mathfrak{H}'$, $\mathfrak{H}' := \ker(I + U_0)^{\perp}$, and $U_0'' = U_0 \upharpoonright \mathfrak{H}'' = -I_{\mathfrak{H}''}$, $\mathfrak{H}'' := \ker(I + U_0)$. One easily verifies that $\ker(I + U_0') = \{0\}$. Hence the construction above can be applied. That means, there is a sequence $\{U_n'\}_{n\in\mathbb{N}}$ of unitary operators with simple pure point spectrum on $\mathfrak{H}'$ such that $U_0' - U_n' \in \mathfrak{L}_1(\mathfrak{H}')$, $n \in \mathbb{N}$, and $\lim_{n\to\infty} \|U_0' - U_n'\|_{\mathfrak{L}_1} = 0$.

On the Hilbert space $\mathfrak{H}''$ we choose $U_n'' = -I$, $n \in \mathbb{N}$. Setting $U_n := U_n' \oplus U_n''$, $n \in \mathbb{N}$, we complete the proof. $\qquad\square$

Proposition 3.4. *Let U_0 be a purely singular unitary operator and let Q be a charge, both acting on the separable Hilbert space $\mathfrak{H}$. Then there is a sequence of unitary operators $\{\widetilde{U}_m\}_{m\in\mathbb{N}}$ and a sequence of bounded self-adjoint operators $\{Q_m\}_{m\in\mathbb{N}}$ both with pure point spectrum such that $[Q_m, \widetilde{U}_m] = 0$ and $U_0 - \widetilde{U}_m \in \mathfrak{L}_1$ for all $m \in \mathbb{N}$ satisfying*

$$\lim_{m\to\infty} \|U_0 - \widetilde{U}_m\|_{\mathfrak{L}_1} = 0 \quad and \quad Q = s\text{-}\lim_{m\to\infty} \widetilde{Q}_m.$$

Proof. By Lemma 3.1 we find a decomposition

$$U_0 = \bigoplus_{k\in\mathbb{N}} U_k \quad \text{and} \quad Q = \bigoplus_{k\in\mathbb{N}} Q_k$$

where U_k is of constant spectral multiplicity and Q_k are bounded self-adjoint operators commuting with U_k such that $\sup_{k\in\mathbb{N}} \|Q_k\|_{\mathfrak{H}_k} = \|Q\|_{\mathfrak{H}}$.

By Lemma 3.2 for each $k \in \mathbb{N}$ there is a sequence $\{Q_{km}\}_{m\in\mathbb{N}}$ of bounded self-adjoint operators with pure point spectrum commuting with U_k such that $\|Q_{km}\|_{\mathfrak{H}_k} \le \|Q_k\|_{\mathfrak{H}} + 1$ for each $m \in \mathbb{N}$ and $Q_k = s\text{-}\lim_{m\to\infty} Q_{km}$. The operators Q_{km} admit the representation

$$Q_{km} = \sum_{l\in\mathbb{N}} \lambda_{kml} P_{kml}$$

where P_{kml} are eigenprojections of Q_{kml} in $\mathfrak{H}_k$. Since U_k commutes with Q_{km} the eigenprojections P_{kml} commute with U_k. We set $U_{kml} := U_k \upharpoonright \mathfrak{H}_{kml}$ where $\mathfrak{H}_{kml} := P_{kml}\mathfrak{H}_k$. Notice that

$$U_{km} = \bigoplus_{l\in\mathbb{N}} U_{kml}.$$

The unitary operators U_{kml} are singular but their spectral multiplicity might be not constant.

By Lemma 3.2 for each $k, m, l \in \mathbb{N}$ there is a unitary operator $\widetilde{U}_{kml}$ on $\mathfrak{H}_{kml}$ such that the spectrum of U_{kml} is pure point, $U_{kml} - \widetilde{U}_{kml} \in \mathfrak{L}_1(\mathfrak{H}_{kml})$ and

$$\|U_{kml} - \widetilde{U}_{kml}\| \le \frac{1}{(k+m+l)^3}.$$

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Obviously, $\widetilde{U}_{kml}$ commutes with P_{kml}. Setting

$$\widetilde{U}_{km} := \bigoplus_{l \in \mathbb{N}} \widetilde{U}_{kml}$$

we get a unitary operator on $\mathfrak{H}_k$ with pure point spectrum which commutes with Q_{km}. Moreover, we have

$$\|U_{km} - \widetilde{U}_{km}\|_{\mathfrak{L}_1} \leq \sum_{l \in \mathbb{N}} \frac{1}{(k+m+l)^3}.$$

Finally, setting

$$\widetilde{U}_m := \bigoplus_{k \in \mathbb{N}} \widetilde{U}_{km} \quad \text{and} \quad Q_m := \bigoplus_{k \in \mathbb{N}} Q_{km}$$

we define a unitary and a self-adjoint operator on $\mathfrak{H}$. Obviously, $\widetilde{U}_m$ and Q_m commute for each $m \in \mathbb{N}$ and they are pure point. Since

$$\|U_0 - \widetilde{U}_m\|_{\mathfrak{L}_1} \leq \sum_{k \in \mathbb{N}} \sum_{l \in \mathbb{N}} \frac{1}{(m+k+l)^3}$$

we have $U_0 - \widetilde{U}_m \in \mathfrak{L}_1(\mathfrak{H})$ for each $m \in \mathbb{N}$ and $\lim_{m \to \infty} \|U_0 - \widetilde{U}_m\|_{\mathfrak{L}_1} = 0$. We recall that $s\text{-}\lim_{m \to \infty} Q_m = Q$ by Lemma 3.1. $\qquad\qquad\square$

Proposition 3.5. *Let $\mathcal{S} = \{U, U_0\}$ be a $\mathfrak{L}_1$-scattering system. Further, let Q be a charge and ρ be a density operator. If $U - U_0$ is trace class, then $J = J_{ac}$ (see (23)), i.e. the pure point and singular continuous spectral subspaces of U_0 do not contribute to the steady current.*

Proof. Using the decompositions $U_0 = U_0^{ac} \oplus U_0^s$ and $Q = Q_{ac} \oplus Q_s$ we have:

$$J = -\frac{1}{2}\text{tr}(\Omega_- \rho U_0^* \Omega_-^* [V, Q_{ac}]) - \frac{1}{2}\text{tr}(\Omega_- \rho U_0^* \Omega_-^* [V, Q_s]).$$

We are going to show that $J_s := -\frac{1}{2}\text{tr}(\Omega_- \rho U_0^* \Omega_-^* [V, Q_s]) = 0$.

Let us first assume that the spectra of U_0^s and Q_s are pure point. Hence U_0^s and Q_s admit the representations

$$U_0^s = \sum_{n \in \mathbb{N}} \zeta_n P_n \quad \text{and} \quad Q_s = \sum_{l \in \mathbb{N}} q_l Q_l$$

where $\zeta_n \in \mathbb{T}$, $q_l \in \mathbb{R}$ and P_n, Q_l are eigenprojections of U_0^s and Q_s, respectively. Since U_0^s and Q_s commute, then their eigenprojections P_n and Q_l also commute. We set $Q_{nl} := P_n Q_l$, which define some orthogonal projections. We have the representation

$$U^s = \sum_{n,l \in \mathbb{N}} \zeta_{nl} Q_{nl} \quad \text{and} \quad Q_s = \sum_{n,l \in \mathbb{N}} q_{nl} Q_{nl}$$

where $\zeta_{nl} \in \mathbb{T}$ and $q_{nl} \in \mathbb{R}$. Notice that $\sum_{n,l \in \mathbb{N}} Q_{nl} = P^s(U_0)$. Without loss of generality we can assume that Q_{nl} are one dimensional orthogonal projections. Because the series $\sum_{n,l \in \mathbb{N}} \zeta_{nl} Q_{nl} [V, Q_{nl}]$ converges in the trace class norm to $[V, Q_s]$, we can write:

$$J^s = -\frac{1}{2} \sum_{n,l \in \mathbb{N}} q_{nl} \text{tr}(\Omega_- \rho U_0^* \Omega_-^* [V, Q_{nl}]).$$

Now we can undo each commutator and write:

$$\text{tr}(\Omega_- \rho \Omega_-^* [V, Q_{nl}]) = \text{tr}(\Omega_- \rho U_0^* \Omega_-^* U Q_{nl}) - \text{tr}(\Omega_- \rho U_0^* \Omega_-^* Q_{nl} U).$$

Using trace cyclicity we have $\text{tr}(\Omega_- \rho U_0^* \Omega_-^* Q_{nl} U) = \text{tr}(U \Omega_- \rho U_0^* \Omega_-^* Q_{nl})$, and then because U commutes with $\Omega_- \rho U_0^* \Omega_-^*$ due to the intertwining property of the wave operator, we can put U at the left of Q_{nl}. Hence $J_s = 0$.

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If U^s and Q_s are not pure point, then in accordance with Proposition 3.4 there is a sequence $\{U_m^s\}_{m\in\mathbb{N}}$ of pure point unitary operators acting on $\mathfrak{H}^s(U_0)$ and a sequence $\{Q_{s,m}\}_{m\in\mathbb{N}}$ of bounded self-adjoint operators with pure point spectrum acting on $\mathfrak{H}^s(U_0)$ such that $[U_m^s, Q_{s,m}] = 0$ and $U_0^s - U_n^s \in \mathfrak{L}_1(\mathfrak{H}^s(U_0))$ for $m \in \mathbb{N}$ as well as $\lim_{m\to\infty} \|U_0^s - U_m^s\|_{\mathfrak{L}_1} = 0$ and $s\text{-}\lim_{m\to\infty} Q_m = Q_s$.

We set
$$U_m := U_0^{ac} \oplus U_m^s \quad \text{and} \quad Q_m := Q_{ac} \oplus Q_{s,m}, \quad m \in \mathbb{N}.$$

We have $[U_m, Q_m] = 0$ and $U_0 - U_m \in \mathfrak{L}_1(\mathfrak{H})$ for $m \in \mathbb{N}$ as well as $\lim_{m\to\infty} \|U_0 - U_m\|_{\mathfrak{L}_1} = 0$ and $s\text{-}\lim_{m\to\infty} Q_m = Q$. Since $U - U_m = U - U_0 + U_0 - U_m \in \mathfrak{L}_1(\mathfrak{H})$ the wave operators
$$\Omega_\pm(U, U_m) = s\text{-}\lim_{n\to\pm\infty} U^n U_m^{-n} P^{ac}(U_m)$$

exist for each $m \in \mathbb{N}$. However, we have $\Omega_\pm = \Omega_\pm(U, U_m)$ for each $m \in \mathbb{N}$ since $U_m^{ac} = U_0^{ac}$. Let
$$J_m := -\frac{1}{2}\operatorname{tr}(\Omega_-(U, U_m)\rho_{ac} U_0^* \Omega_-(U, U_m)^* [V_m, Q_m]), \quad m \in \mathbb{N},$$

where $V_m := U - U_m$. We note that $J_m = (J_m)_{ac} + (J_m)_s$ where

$$
\begin{aligned}
(J_m)_{ac} &:= -\frac{1}{2}\operatorname{tr}(\Omega_-(U, U_m)\rho_{ac} U_0^* \Omega_\pm(U, U_m)^* [V_m, Q_{ac}]) \\
(J_m)_s &:= -\frac{1}{2}\operatorname{tr}(\Omega_-(U, U_m)\rho_{ac} U_0^* \Omega_\pm(U, U_m)^* [V_m, Q_{s,m}]).
\end{aligned}
$$

Since U_m^s and $Q_{s,m}$ are pure point we get by the considerations above that $(J_m)_s = 0$ for each $m \in \mathbb{N}$. Hence $J_m = (J_m)_{ac}, m \in \mathbb{N}$.

Furthermore, using $\Omega_\pm = \Omega_\pm(U, U_m)$ and $U_0^{ac} = U_m^{ac}$ we find
$$J_m = (J_m)_{ac} = -\frac{1}{2}\operatorname{tr}(\Omega_- \rho_{ac} U_0^* \Omega_-^* [V_m, Q_{ac}]), \quad m \in \mathbb{N}.$$

Since $\lim_{m\to\infty} \|U_0 - U_m\|_{\mathfrak{L}_1} = 0$ and $s\text{-}\lim_{m\to\infty} Q_m = Q$ we find $\lim_{m\to\infty} J_m = J$ and $\lim_{m\to\infty} (J_m)_{ac} = J_{ac}$ which yields $J = J_{ac}$. $\qquad\square$

Lemma 3.6. *Let $\{U, U_0\}$ be a $\mathfrak{L}_1$-scattering system. With the notation introduced in (91), let*
$$J(r) := -\frac{1}{2}\operatorname{tr}(\Omega_-(r)\rho U_0^* \Omega_-(r)^* [V, Q_{ac}]), \quad r \in [0, 1).$$

If $\sigma_s(U) = \emptyset$, then $J = \lim_{r\uparrow 1} J(r)$.

Proof. We set
$$J^{ac}(r) := -\frac{1}{2}\operatorname{tr}(\Omega_-(r)\rho U_0^* \Omega_-(r)^* P^{ac}(U)[V, Q_{ac}])$$

and
$$J^s(r) := -\frac{1}{2}\operatorname{tr}(\Omega_-(r)\rho U_0^* \Omega_-(r)^* P^s(U)[V, Q_{ac}]).$$

Since $\Omega_-^* = s\text{-}\lim_{r\uparrow 1} \Omega_-(r)^* P^{ac}(U)$ one easily verifies that $J = \lim_{r\uparrow} J^{ac}(r)$.

Let us show that $\lim_{r\uparrow 1} J^s(r) = 0$. To this end we verify that
$$s\text{-}\lim_{r\uparrow 1} \Omega_-(r)^* P^s(U) = 0.$$

Let $\varphi_k, \|\varphi_k\| = 1$, be an eigenvector of U corresponding to the eigenvalue $\xi_k \in \mathbb{T}$. One gets
$$\Omega_-(r)^* \varphi_k = (1-r) P_0^{ac} \sum_{n\in\mathbb{N}} r^k U_0^{-n} U^n \varphi_k = (1-r) P_0^{ac} \sum_{n\in\mathbb{N}} r^k U_0^{-n} \xi_k^n \varphi_k.$$

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Hence

$$\Omega_-(r)^*\varphi_k = P_0^{ac} \frac{1-r}{I - U_0^*\xi_k}\varphi_k = (1-r)\int_{\mathbb{T}} \frac{1}{1 - r\overline{\zeta}\xi}dE_0^{ac}(\zeta)\varphi_k.$$

We introduce the Borel subset Δ_k^N of $\mathbb{T}$ defined by

$$\Delta_k^N := \left\{ \zeta \in \mathbb{T} : \frac{d(E_0^{ac}(\zeta)\varphi_k,\varphi_k)}{d\nu(\zeta)} \leq N \right\}. \tag{25}$$

It is not hard to see that $s\text{-}\lim_{N\to\infty} E_0^{ac}(\mathbb{T} \setminus \Delta_k^N) = 0$. By the decomposition

$$\Omega_-(r)^*\varphi_k = (1-r)\int_{\Delta_k^N} \frac{1}{1 - r\overline{\zeta}\xi_k}dE_0^{ac}(\zeta)\varphi_k +$$
$$(1-r)\int_{\mathbb{T}\setminus\Delta_k^N} \frac{1}{1 - r\overline{\zeta}\xi}dE_0^{ac}(\zeta)\varphi_k$$

we find

$$\|\Omega_-(r)^*\varphi_k\|^2 = \frac{1-r}{1+r}\int_{\Delta_k^N} \frac{1-r^2}{|1 - r\overline{\zeta}\xi_k|^2}\frac{d(E_0^{ac}(\zeta)\varphi_k,\varphi_k)}{d\nu(\zeta)} +$$
$$(1-r)^2\int_{\mathbb{N}\setminus\Delta_k^N} \frac{1}{|1 - r\overline{\zeta}\xi_k|^2}\frac{d(E_0^{ac}(\zeta)\varphi_k,\varphi_k)}{d\nu(\zeta)}.$$

Taking into account (25) we find the estimate

$$\|\Omega_-(r)^*\varphi_k\|^2 \leq 2\pi N\frac{1-r}{1+r} + (1-r)^2\int_{\mathbb{N}\setminus\Delta_k^N} \frac{1}{|1 - r\overline{\zeta}\xi_k|^2}\frac{d(E_0^{ac}(\zeta)\varphi_k,\varphi_k)}{d\nu(\zeta)}.$$

Using $\frac{(1-r)^2}{|1-r\overline{\zeta}\xi_k|^2} \leq 1$ we get

$$\|\Omega_-(r)^*\varphi_k\|^2 \leq 2\pi N\frac{1-r}{1+r} + (E_0^{ac}(\mathbb{T} \setminus \Delta_k^N)\varphi_k,\varphi_k).$$

For each $\varepsilon > 0$ there is N_0 such that $(E_0^{ac}(\mathbb{T} \setminus \Delta_k^N)\varphi_k,\varphi_k) < \frac{\varepsilon}{2}$ for $N > N_0$. Fixing such a N there is $r_0 < 1$ such that for $r \in (r_0, 1)$ one has $2\pi N\frac{1-r}{1+r} < \frac{\varepsilon}{2}$.

$$\|\Omega_-(r)^*\varphi_k\|^2 \leq \varepsilon.$$

Hence $\lim_{r\uparrow 1} \|\Omega_-(r)^*\varphi_k\|^2 = 0$. From the above considerations we get $\lim_{r\uparrow 1} \Omega_-^*(r)f = 0$ provided $f = \sum_k c_k f_k$, $c_k \in \mathbb{C}$, is a finite sum of eigenvectors of U. However, the set of finite sums of eigenvectors of U is dense in $\mathfrak{H}^s(U)$ which yields $s\text{-}\lim_{r\uparrow 1} \Omega_-^*(r)P^s(U) = 0$. Using $s\text{-}\lim_{r\uparrow 1} \Omega_-(r) = \Omega_-$ and the compactness of V we immediately get that $\lim_{r\uparrow 1} J^s(r) = 0$. $\qquad\square$

Using the results above we are now going to prove a Landauer-Büttiker formula for unitary operators

Theorem 3.7. *Let $\mathcal{S} = \{U, U_0\}$ be a $\mathfrak{L}_1$-scattering system. Further let Q_0 be a charge and let ρ be a density operator. If $\sigma_{sc}(U) = \emptyset$, then*

$$J = \frac{1}{4\pi}\int_{\mathbb{T}} \text{tr}\{\rho_{ac}(\zeta)[Q_{ac}(\zeta) - S(\zeta)^*Q_{ac}(\zeta)S(\zeta)]\}\,d\nu(\zeta) \tag{26}$$

where $S(\zeta)$ is the scattering matrix of the scattering system $\mathcal{S}$.

Proof. Let us introduce the approximate current by

$$J(r,\varepsilon) := -\frac{1}{2}\text{tr}(\Omega_-(r)\rho_{ac}^\varepsilon U_0^*\Omega_-(r)^*[V, Q_{ac}]), \quad 0 \leq r < 1,$$

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where

$$\rho_{ac}^{\varepsilon} := E_0^{ac}(\Delta_*(\varepsilon))\rho, \qquad \varepsilon \geq 0, \tag{27}$$

and $\Delta_*(\varepsilon) \subseteq \mathbb{T}$ satisfying $\nu(\Delta_*(\varepsilon)) < \varepsilon$ and (112). Notice that ρ_{ac}^{ε} is also a density operator. By Lemma 3.6 we immediately get that $\lim_{r\uparrow 1} J(r,\varepsilon) = J(\varepsilon)$ where

$$J(\varepsilon) := -\frac{1}{2}\mathrm{tr}(\Omega_- \rho_{ac}^{\varepsilon} U_0^* \Omega_-^* [V, Q_{ac}]).$$

Furthermore, we note that

$$J = \lim_{\varepsilon\to+0} J(\varepsilon) = \lim_{\varepsilon\to+0} \lim_{r\uparrow 1} J(r,\varepsilon) \tag{28}$$

where J is given by (22). We set

$$\begin{aligned} J_1(\varepsilon) &:= \mathrm{tr}(\rho_{ac}^{\varepsilon} \Omega_-^* V Q_{ac} \Omega_- U_0^*), \\ J_2(\varepsilon) &:= \mathrm{tr}(\rho_{ac}^{\varepsilon} U_0^* \Omega_-^* Q_{ac} V \Omega_-) \end{aligned}$$

and

$$\begin{aligned} J_1(r,\varepsilon) &:= \mathrm{tr}(\rho_{ac}^{\varepsilon} \Omega_-(r)^* V Q_{ac} \Omega_-(r) U_0^*), \\ J_2(r,\varepsilon) &:= \mathrm{tr}(\rho_{ac}^{\varepsilon} \Omega_-(r)^* Q_{ac} U_0 V \Omega_-(r)), \end{aligned} \qquad 0 \leq r < 1.$$

Notice that

$$\begin{aligned} -2J(\varepsilon) &= J_1(\varepsilon) - J_2(\varepsilon) \\ -2J(r,\varepsilon) &= J_1(r,\varepsilon) - J_2(r,\varepsilon), \end{aligned} \tag{29}$$

$0 \leq r < 1$. Setting $K(r) := \Omega_-(r)^* V$, $0 \leq r < 1$, we get

$$J_1(r,\varepsilon) = \mathrm{tr}(\rho_{ac}^{\varepsilon} K(r) Q_{ac} \Omega_- U_0^*),$$

Using $V = -U_0 V^* U$ we obtain which yields

$$J_2(r,\varepsilon) := -\mathrm{tr}(\rho_{ac}^{\varepsilon} \Omega_-(r)^* Q_{ac} U_0 K(r)^*). \tag{30}$$

At first, we are going to calculate $K(r)Q_{ac}\Omega_-(r)U_0^*$. From (93) we get

$$K(r)Q_{ac}\Omega_-(r)U_0^* = K(r)Q_{ac}\left\{ P_0^{ac} + r\int_{\mathbb{T}} \frac{1}{I - r\zeta U^*} V^* U_0 dE_0^{ac}(\zeta) \right\} U_0^*$$

where we have used $U^* V = -V^* U_0$ which leads to

$$K(r)Q_{ac}\Omega_-(r)U_0^* = K(r)Q_{ac}\left\{ U_0^* P_0^{ac} + r\int_{\mathbb{T}} \frac{1}{I - r\zeta U^*} V^* dE_0^{ac}(\zeta) \right\}.$$

Setting

$$\Xi(r) := r\int_{\mathbb{T}} \frac{1}{I - r\zeta U^*} V^* dE_0^{ac}(\zeta) \tag{31}$$

we get

$$K(r)Q_{ac}\Omega_-(r)U_0^* = K(r)Q_{ac}U_0^* P_0^{ac} + K(r)Q_{ac}\Xi(r)$$

and

$$J_1(r,\epsilon) = \mathrm{tr}(\rho_{ac}^{\varepsilon} K(r) Q_{ac} U_0^*) + \mathrm{tr}(\rho_{ac}^{\varepsilon} K(r) Q_{ac} \Xi(r)).$$

Using the unitary operator Φ and (107) we find

$$(\Phi K(r) Q_{ac} U_0^* \Phi^{-1} \widehat{f})(\zeta) = \int_{\mathbb{T}} K(r;\zeta,\zeta') Q_{ac}(\zeta') \overline{\zeta'} \widehat{f}(\zeta') d\nu(\zeta'),$$

$\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. By the resolvent formula one has the identity

$$(I - \xi U^*)^{-1} = (I - \xi U_0^*)^{-1} \left\{ I + \zeta V^* (I - \xi U^*)^{-1} \right\}, \quad \xi \in \mathbb{D}.$$

Multiplying on the right by V^* we get

$$(I - \xi U^*)^{-1} V^* = (I - \xi U_0^*)^{-1} \left\{ V^* + \xi V^* (I - \xi U^*)^{-1} V^* \right\}, \quad \xi \in \mathbb{D},$$

which yields

$$(I - \xi U^*)^{-1} V^* = (I - \xi U_0^*)^{-1} C Z(\xi) C, \quad \xi \in \mathbb{D}.$$

Using that we obtain

$$\Xi(r) = r \int_{\mathbb{T}} (I - r\zeta' U_0^*)^{-1} C Z(r\zeta') C dE_0^{ac}(\zeta')$$

which yields

$$\Xi(r) = r \int_{\mathbb{T}} E_0^{ac}(d\xi) C \int_{\mathbb{T}} (I - r\zeta' \overline{\xi})^{-1} Z(r\zeta') C dE_0^{ac}(\zeta'). \tag{32}$$

Applying the map Φ one gets

$$(\Phi \Xi(r) \Phi^{-1} \widehat{f})(\xi) = r \sqrt{Y(\xi)} \int_{\mathbb{T}} (I - r\zeta' \overline{\xi})^{-1} Z(r\zeta') \sqrt{Y(\zeta')} \, \widehat{f}(\zeta') d\nu(\zeta').$$

or

$$(\Phi \Xi(r) \Phi^{-1} \widehat{f})(\xi) = r \int_{\mathbb{T}} (I - r\zeta' \overline{\xi})^{-1} K(r; \zeta', \xi)^* \, \widehat{f}(\zeta') d\nu(\zeta'),$$

$\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. Using

$$(\Phi K(r) Q_{ac} \Xi(r) \Phi^{-1} \widehat{f})(\xi) = (\Phi K(r) \Phi^{-1} \Phi Q_{ac} \Phi^{-1} \Phi \Xi(r) \Phi^{-1} \widehat{f})(\xi)$$

and (107) we find

$$(\Phi K(r) Q_{ac} \Xi(r) \Phi^{-1} \widehat{f})(\zeta) =$$
$$r \int_{\mathbb{T}} d\nu(\xi) K(r; \zeta, \xi) Q_{ac}(\xi) \int_{\mathbb{T}} d\nu(\zeta')(I - r\zeta' \overline{\xi})^{-1} K(r; \zeta', \xi)^* \, \widehat{f}(\zeta').$$

Setting

$$
\begin{aligned}
M(r; \zeta, \xi, \zeta') &:= K(r; \zeta, \xi) Q_{ac}(\xi) K(r; \zeta', \xi)^* \\
&= \sqrt{Y(\zeta)} Z(r\zeta)^* \sqrt{Y(\xi)} Q_{ac}(\xi) \sqrt{Y(\xi)} Z(r\zeta') \sqrt{Y(\zeta')} \\
&= X_*(r; \zeta) \sqrt{Y(\xi)} Q_{ac}(\xi) \sqrt{Y(\xi)} X_*(r; \overline{\zeta'})^*
\end{aligned}
\tag{33}
$$

we find

$$(\Phi K(r) Q_{ac} \Xi(r) \Phi^{-1} \widehat{f})(\zeta) = r \int_{\mathbb{T}} d\nu(\xi) \int_{\mathbb{T}} d\nu(\zeta') \frac{M(r; \zeta, \xi, \zeta')}{I - r\zeta' \overline{\xi}} \, \widehat{f}(\zeta')$$

where $X_*(r; \zeta)$ is defined by (111). Notice that

$$M(r; \zeta, \xi, \zeta')^* = M(r; \zeta', \xi, \zeta).$$

Summing up we obtain

$$
\begin{aligned}
J_1(r, \varepsilon) = &\int_{\mathbb{T}} d\nu(\zeta) \overline{\zeta} \operatorname{tr}(\rho_{ac}^\varepsilon(\zeta) K(r; \zeta, \zeta) Q_{ac}(\zeta)) + \\
&r \int_{\mathbb{T}^2} d\nu(\zeta) d\nu(\xi) \operatorname{tr}\left(\rho_{ac}^\varepsilon(\zeta) \frac{M(r; \zeta, \xi, \zeta)}{I - r\zeta \overline{\xi}} \right).
\end{aligned}
\tag{34}
$$

We are going to calculate $J_2(r, \varepsilon)$. From (96) we get

$$\Omega_-(r)^* Q_{ac} U_0 K(r)^* = \left\{ P_0^{ac} + r \int_{\mathbb{R}} dE_0^{ac}(\zeta) V \frac{\overline{\zeta}}{I - r\overline{\zeta} U} \right\} Q_{ac} U_0 K(r)^*$$

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or

$$\Omega_-(r)^* Q_{ac} U_0 K(r)^* = Q_{ac} U_0 K(r)^* + r \int_{\mathbb{R}} dE_0^{ac}(\zeta) V \frac{\overline{\zeta}}{I - r\overline{\zeta} U} Q_{ac} U_0 K(r)^*$$

which yields

$$\Omega_-(r)^* Q_{ac} U_0 K(r)^* = Q_{ac} U_0 K(r)^* + r U_0^* \int_{\mathbb{R}} dE_0^{ac}(\zeta) V \frac{1}{I - r\overline{\zeta} U} Q_{ac} U_0 K(r)^*.$$

Using the notation (31) we obtain

$$\Omega_-(r)^* Q_{ac} U_0 K(r)^* = Q_{ac} U_0 K(r)^* + r U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^*. \tag{35}$$

Obviously we have

$$(\Phi Q_{ac} U_0 K(r)^* \Phi^{-1} \widehat{f})(\zeta) = Q_{ac}(\zeta) \zeta \int_{\mathbb{T}} K(r; \xi, \zeta)^* \widehat{f}(\xi) d\nu(\xi), \tag{36}$$

$\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. Using (32) we find

$$U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^* = r U_0^* \int_{\mathbb{T}} dE_0^{ac}(\zeta) CZ(r\zeta)^* \int_{\mathbb{T}} C dE_0^{ac}(\xi)(1 - r\overline{\zeta}\xi)^{-1} Q_{ac} U_0 K(r)^*$$

which yields

$$(\Phi U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^* \Phi^{-1} \widehat{f})(\zeta)$$
$$= r \left(\Phi U_0^* \int_{\mathbb{T}} dE_0^{ac}(\zeta) CZ(r\zeta)^* \Phi^{-1} \Phi \int_{\mathbb{T}} C dE_0^{ac}(\xi)(1 - r\overline{\zeta}\xi)^{-1} \Phi^{-1} \Phi Q_{ac} U_0 K(r)^* \Phi^{-1} \widehat{f} \right)(\zeta),$$

Hence

$$(\Phi U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^* \Phi^{-1} \widehat{f})(\zeta)$$
$$= r\overline{\zeta} \sqrt{Y(\zeta)} Z(r\zeta)^* \int_{\mathbb{T}} d\nu(\xi) \sqrt{Y(\xi)}(1 - r\overline{\zeta}\xi)^{-1} Q_{ac}(\xi) \xi \int_{\mathbb{T}} d\nu(\zeta') K(r; \zeta', \xi)^* \widehat{f}(\zeta').$$

Since $K(r; \zeta, \xi) := \sqrt{Y(\zeta)} Z(r\zeta)^* \sqrt{Y(\xi)}$ by definition we get

$$(\Phi U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^* \Phi^{-1} \widehat{f})(\zeta) =$$
$$r \int_{\mathbb{T}} d\nu(\xi) \frac{\overline{\zeta}\xi K(r; \zeta, \xi)}{1 - r\overline{\zeta}\xi} Q_{ac}(\xi) \int_{\mathbb{T}} d\nu(\zeta') K(r; \zeta', \xi)^* \widehat{f}(\zeta'),$$

Finally, by definition (33) we find

$$(\Phi U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^* \Phi^{-1} \widehat{f})(\zeta) = \int_{\mathbb{T}} d\nu(\xi) \int_{\mathbb{T}} d\nu(\zeta') \frac{\overline{\zeta}\xi M(r; \zeta, \xi, \zeta')}{1 - r\overline{\zeta}\xi} \widehat{f}(\zeta'). \tag{37}$$

From (30) and (35) it follows

$$J_2(r, \varepsilon) = -\text{tr}(\rho_{ac}^{\varepsilon} Q_{ac} U_0 K(r)^*) - r\text{tr}(\rho_{ac}^{\varepsilon} U_0^* \Xi(r)^* Q_{ac} U_0 K(r)^*).$$

Taking into account (36) and (37) we obtain

$$J_2(r, \varepsilon) = -\int_{\mathbb{T}} d\nu(\zeta) \zeta \text{tr}(\rho_{ac}^{\varepsilon}(\zeta) Q_{ac}(\zeta) K(r; \zeta, \zeta)^*) \tag{38}$$
$$- r \int_{\mathbb{T}} \int_{\mathbb{T}} d\nu(\zeta) d\nu(\xi) \frac{\overline{\zeta}\xi}{1 - r\overline{\zeta}\xi} \text{tr}(\rho_{ac}^{\varepsilon}(\zeta) M(r; \zeta, \xi, \zeta)).$$

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From (29), (34) and (38) we get

$$-2J(r,\varepsilon) = \int_{\mathbb{T}} d\nu(\zeta)\overline{\zeta}\,\mathrm{tr}\,(\rho_{ac}^{\varepsilon}(\zeta)K(r;\zeta,\zeta)Q_{ac}(\zeta))$$

$$+ \int_{\mathbb{T}} d\nu(\zeta)\zeta\,\mathrm{tr}\,(\rho_{ac}^{\varepsilon}(\zeta)Q_{ac}(\zeta)K(r;\zeta,\zeta)^{*})$$

$$+ r\int_{\mathbb{T}} d\nu(\zeta) \int_{\mathbb{T}} d\nu(\xi) \left\{ \frac{1}{I - r\zeta\overline{\xi}} + \frac{\overline{\zeta}\xi}{1 - r\overline{\zeta}\xi} \right\} \mathrm{tr}\,(\rho_{ac}^{\varepsilon}(\zeta)M(r;\zeta,\xi,\zeta))$$

which yields

$$-2J(r,\varepsilon) = \int_{\mathbb{T}} d\nu(\zeta)\overline{\zeta}\,\mathrm{tr}\,(\rho_{ac}^{\varepsilon}(\zeta)K(r;\zeta,\zeta)Q_{ac}(\zeta))$$

$$+ \int_{\mathbb{T}} d\nu(\zeta)\zeta\,\mathrm{tr}\,(\rho_{ac}^{\varepsilon}(\zeta)Q_{ac}(\zeta)K(r;\zeta,\zeta)^{*})$$

$$+ 2\pi\frac{r}{1+r}\frac{1-r^2}{2\pi} \int_{\mathbb{T}} d\nu(\zeta) \int_{\mathbb{T}} d\nu(\xi)\frac{1+\overline{\zeta}\xi}{|I - r\zeta\overline{\xi}|^2}\mathrm{tr}\,(\rho_{ac}^{\varepsilon}(\zeta)M(r;\zeta,\xi,\zeta)).$$

By (27) we get

$$-2J(r,\varepsilon) = \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\overline{\zeta}\,\mathrm{tr}\,(\rho_{ac}(\zeta)K(r;\zeta,\zeta)Q_{ac}(\zeta))$$

$$+ \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\zeta\,\mathrm{tr}\,(\rho_{ac}(\zeta)Q_{ac}(\zeta)K(r;\zeta,\zeta)^{*})$$

$$+ 2\pi\frac{r}{1+r}\frac{1-r^2}{2\pi} \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta) \int_{\mathbb{T}} d\nu(\xi)\frac{1+\overline{\zeta}\xi}{|I - r\zeta\overline{\xi}|^2}\mathrm{tr}\,(\rho_{ac}(\zeta)M(r;\zeta,\xi,\zeta)).$$

Using the representation $K(r;\zeta,\zeta) = X_*(r;\zeta)\sqrt{Y(\zeta)}$ and taking into account (112) we find that

$$\lim_{r\uparrow 1} \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\overline{\zeta}\,\mathrm{tr}\,(\rho_{ac}(\zeta)K(r;\zeta,\zeta)Q_{ac}(\zeta)) = \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\overline{\zeta}\,\mathrm{tr}\,(\rho_{ac}(\zeta)K(\zeta,\zeta)Q_{ac}(\zeta))$$

and

$$\lim_{r\uparrow 1} \int_{\mathbb{T}} d\nu(\zeta)\zeta\,\mathrm{tr}\,(\rho_{ac}(\zeta)Q_{ac}(\zeta)K(r;\zeta,\zeta)^{*}) = \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\zeta\,\mathrm{tr}\,(\rho_{ac}(\zeta)Q_{ac}(\zeta)K(\zeta,\zeta)^{*}).$$

Furthermore, using (33) we find that

$$\frac{1-r^2}{2\pi} \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta) \int_{\mathbb{T}} d\nu(\xi)\frac{1+\overline{\zeta}\xi}{|I - r\zeta\overline{\xi}|^2}\mathrm{tr}\,(\rho_{ac}(\zeta)M(r;\zeta,\xi,\zeta))$$

$$= \int_{\mathbb{T}} d\nu(\xi)\frac{1-r^2}{2\pi} \int_{\mathbb{T}} d\nu(\zeta)\frac{1+\overline{\zeta}\xi}{|I - r\zeta\overline{\xi}|^2}F(r;\zeta,\xi)\chi_{\mathbb{T}\backslash\Delta(\varepsilon)}(\zeta)$$

where

$$F(r;\zeta,\xi) := \mathrm{tr}\,\left(\rho_{ac}(\zeta)X_*(r;\zeta)\sqrt{Y(\xi)}Q_{ac}(\xi)\sqrt{Y(\xi)}X_*(r;\overline{\zeta})^{*}\right)$$

$\zeta \in \mathbb{T}\setminus\Delta_*(\varepsilon), \xi \in \mathbb{T}$ and $0 \leq r < 1$. By (112) we get the estimate

$$|F(r;\zeta,\xi)| \leq C_{X_*}(\varepsilon)^2\|\rho_{ac}\|\|Q_{ac}\|\mathrm{tr}(Y(\xi)),\ \zeta \in \mathbb{T}\setminus\Delta_*(\varepsilon)),\ 0 \leq r < 1,\ \xi \in \mathbb{T}.$$

Hence

$$\left| \frac{1-r^2}{2\pi} \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\frac{1+\overline{\zeta}\xi}{|I - r\zeta\overline{\xi}|^2}F(r;\zeta,\xi) \right| \leq$$

$$2\frac{1-r^2}{2\pi} \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\frac{1}{|I - r\zeta\overline{\xi}|^2}|F(r;\zeta,\xi)| \leq 2C_{X_*}(\varepsilon)^2\|\rho_{ac}\|\|Q_{ac}\|\mathrm{tr}(Y(\xi))$$

where $\mathrm{tr}(Y(\xi)) \in L^1(\mathbb{T}, d\nu(\xi))$. Applying the Lebesgue dominated convergence theorem we obtain

$$\frac{1-r^2}{2\pi} \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta) \int_\mathbb{T} d\nu(\xi) \frac{1 + \overline{\zeta}\xi}{|I - r\zeta\overline{\xi}|^2} \mathrm{tr}\left(\rho_{ac}(\zeta)M(r;\zeta,\xi,\zeta)\right)$$

$$= \int_\mathbb{T} d\nu(\xi)F(\xi,\xi)\chi_{\mathbb{T}\backslash\Delta(\varepsilon)}(\xi) = \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\xi)F(\xi,\xi)$$

where

$$F(\xi,\xi) := \mathrm{tr}\left(\rho_{ac}(\xi)X_*(\xi)\sqrt{Y(\xi)}Q_{ac}(\xi)\sqrt{Y(\xi)}X_*(\overline{\xi})^*\right) = \mathrm{tr}(\rho_{ac}(\xi)M(\xi,\xi,\xi))$$

and $M(\zeta,\zeta,\zeta) = \mathfrak{L}_1 - \lim_{r\uparrow 1} M(r;\zeta,\zeta,\zeta)$ for a.e. $\xi \in \mathbb{T}$. Summing up we obtain

$$\begin{aligned} -2J(\varepsilon) := 2\lim_{r\uparrow 1} J(r,\varepsilon) &= \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\overline{\zeta}\mathrm{tr}\left(\rho_{ac}(\zeta)K(\zeta,\zeta)Q_{ac}(\zeta)\right) \\ &+ \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\zeta\mathrm{tr}\left(\rho_{ac}(\zeta)Q_{ac}(\zeta)K(\zeta,\zeta)^*\right) \\ &+ 2\pi \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\mathrm{tr}\left(\rho_{ac}(\zeta)M(r;\zeta,\zeta,\zeta)\right). \end{aligned}$$

By Corollary D.3 we verify that

$$\begin{aligned} -2J(\varepsilon) = i\int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\mathrm{tr}\left(\rho_{ac}(\zeta)T(\zeta)^*Q_{ac}(\zeta)\right) \\ - i\int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\mathrm{tr}\left(\rho_{ac}(\zeta)Q_{ac}(\zeta)T(\zeta)\right) + 2\pi \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\mathrm{tr}\left(\rho_{ac}(\zeta)M(\zeta,\zeta,\zeta)\right). \end{aligned}$$

Since $M(\zeta,\zeta,\zeta) = K(\zeta,\zeta)Q_{ac}(\zeta)K(\zeta,\zeta)^*$ one gets $M(\zeta,\zeta,\zeta) = T(\zeta)^*Q_{ac}T(\zeta)$. Therefore

$$2J(\varepsilon) = \int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} d\nu(\zeta)\mathrm{tr}\left(\rho_{ac}(\zeta)\Sigma(\zeta)\right)$$

where

$$\Sigma(\zeta) := -iT(\zeta)^*Q_{ac}(\zeta) + iQ_{ac}(\zeta)T(\zeta) - 2\pi T(\zeta)^*Q_{ac}(\zeta)T(\zeta), \quad \zeta \in \mathbb{T}. \tag{39}$$

Using (109) we obtain $\|\Sigma\|_{\mathfrak{L}_1} \in L^1(\mathbb{T}, d\nu(\zeta))$. Moreover, from (101) we get

$$T(\zeta) = \frac{I_{\mathfrak{h}(\lambda)} - S(\zeta)}{2\pi i} \quad \text{and} \quad T(\zeta)^* = -\frac{I_{\mathfrak{h}(\lambda)} - S(\zeta)^*}{2\pi i}. \tag{40}$$

Inserting (40) into (39) we find

$$\begin{aligned} \Sigma(\zeta) := \frac{I_{\mathfrak{h}(\zeta)} - S(\zeta)^*}{2\pi}Q_{ac}(\zeta) + Q_{ac}(\zeta)\frac{I_{\mathfrak{h}(\zeta)} - S(\zeta)}{2\pi} + \\ 2\pi\frac{I_{\mathfrak{h}(\lambda)} - S(\zeta)^*}{2\pi i}Q_{ac}(\zeta)\frac{I_{\mathfrak{h}(\lambda)} - S(\zeta)}{2\pi i} \end{aligned}$$

which yields

$$\Sigma(\zeta) = \frac{1}{2\pi}\left\{Q_{ac}(\zeta) - S(\zeta)^*Q_{ac}(\zeta)S(\zeta)\right\}.$$

which proves

$$J(\varepsilon) = \frac{1}{4\pi}\int_{\mathbb{T}\backslash\Delta_*(\varepsilon)} \mathrm{tr}\left(\rho_{ac}(\zeta)(Q_{ac}(\zeta) - S(\zeta)^*Q_{ac}(\zeta)S(\zeta))\right)d\nu(\zeta)$$

Using $\|\Sigma(\zeta)\|_{\mathfrak{L}_1} \in L^1(\mathbb{T}, d\nu(\zeta))$ and (28) we immediately prove (26). $\qquad\square$

Corollary 3.8. *If the assumptions of Theorem 3.7 are satisfied, then*

$$J = \frac{1}{4\pi}\int_\mathbb{T} \mathrm{tr}\left((\rho_{ac}(\zeta) - S(\zeta)\rho_{ac}(\zeta)S(\zeta)^*)Q_{ac}(\zeta)\right). \tag{41}$$

Further, let $\phi : \mathbb{T} \longrightarrow [0, \infty)$ be Borel measurable and bounded. If $\rho = \phi(U_0)$, then $J = 0$.

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Proof. Using the fact that $S(\zeta) - I_{\mathfrak{h}(\zeta)} \in \mathfrak{L}_1(\mathfrak{h}(\zeta))$ for a.e $\zeta \in \mathbb{T}$ with respect to ν one immediately shows that (41) follows from (26).

If $\rho = \phi(U_0)$, then $\rho_{ac} = \phi(U_0^{ac})$ which yields $\rho_{ac}(\zeta) = \phi(\zeta)I_{\mathfrak{h}(\zeta)}$ for a.e. $\zeta \in \mathbb{T}$ with respect to ν. Inserting $\rho_{ac}(\zeta) = \phi(\zeta)I_{\mathfrak{h}(\zeta)}$ into (41) we prove $J = 0$. $\qquad\square$

3.2 Self-adjoint operators

Let H_0 and H be self-adjoint operators on the separable Hilbert space $\mathfrak{H}$. If the condition

$$(H + i)^{-1} - (H_0 + i)^{-1} \in \mathfrak{L}_1(\mathfrak{H}) \tag{42}$$

is satisfied, then the pair $\mathcal{S}' = \{H, H_0\}$ is called a $\mathfrak{L}_1$-scattering system. If $\mathcal{S}' = \{H, H_0\}$ is a $\mathfrak{L}_1$-scattering system, then the wave operators

$$W_\pm := \text{s-}\lim_{t \to \pm\infty} e^{itH}e^{-itH_0}P^{ac}(H_0)$$

exist and are complete. The scattering operator is defined by $S' := W_+^* W_-$.

A bounded self-adjoint operator Q commuting with H_0 is called a charge for $\mathcal{S}'$. A non-negative bounded operator ρ commuting with H_0 is called a density operator for $\mathcal{S}'$. To define the current J' for $\mathcal{S}'$ we assume that $(I + H_0^2)\rho$ is a bounded operator. Under this assumption the current J' is defined by

$$J' := -i\operatorname{tr}\left(W_-(I + H_0^2)\rho W_-^*(H - i)^{-1}[H, Q](H + i)^{-1}\right). \tag{43}$$

Using (21) we have that $(H - i)^{-1}[H, Q'](H + i)^{-1} \in \mathfrak{L}_1(\mathfrak{H})$ which shows that the current is well defined. The definition (43) is in accordance with [1]. Indeed, from definition (43) we formally get $J' = -i\operatorname{tr}(W_-\rho W_-^*[H, Q])$.

Theorem 3.9. *Let $\mathcal{S}' = \{H, H_0\}$ be a $\mathfrak{L}_1$-scattering system. Further, let Q be a charge and let ρ be a density operator for $\mathcal{S}'$ such that $(I + H_0^2)\rho$ is a bounded operator. Further, let $\Pi(H_0^{ac})$ a spectral representation of H_0^{ac} such that Q_{ac} and ρ_{ac} are represented by multiplication operators $M_{Q'_{ac}}$ and $M_{\rho'_{ac}}$ induced by the measurable families $\{Q'_{ac}(\lambda)\}_{\lambda \in \mathbb{R}}$ and $\{\rho'_{ac}(\lambda)\}_{\lambda \in \mathbb{R}}$, respectively. If $\sigma_{sc}(H) = \emptyset$, then*

$$J' = \frac{1}{2\pi}\int_{\mathbb{R}} \operatorname{tr}\left(\rho'_{ac}(\lambda)(Q'_{ac}(\lambda) - S'(\lambda)^* Q'_{ac}(\lambda)S'(\lambda))\right) d\lambda \tag{44}$$

where $\{S'(\lambda)\}_{\lambda \in \mathbb{R}}$ is the scattering matrix with respect to the spectral representation $\Pi(H_0^{ac})$.

Proof. Let us introduce the Cayley transforms

$$U := (i - H)(i + H)^{-1} \quad \text{and} \quad U_0 := (i - H_0)(i + H_0)^{-1}.$$

The pair $\mathcal{S} = \{U, U_0\}$ is a $\mathfrak{L}_1$-scattering system if and only if $\mathcal{S}'$ is $\mathfrak{L}_1$-scattering system. By the invariance principle for wave operators one verifies that $W_\pm = \Omega_\pm$ which yields $S = S'$. Obviously, Q is a charge for $\mathcal{S}$ and ρ is a density operator for $\mathcal{S}$. A straightforward computation (compare with (12)) shows that

$$J' = -\frac{1}{2}\operatorname{tr}(\Omega_-\rho U_0^* \Omega_-^*[V, Q]) = -i\operatorname{tr}\left(W_-\rho W_-^*(H - i)^{-1}[H, Q](H + i)^{-1}\right). \tag{45}$$

Let $\Pi(U_0^{ac})$ be the spectral representation of Appendix B. Assume that the operators Q_{ac}, ρ_{ac} and $S = \Omega_+^* \Omega_-$ are represented in $\Pi(U_0^{ac})$ by the multiplication operators $M_{Q_{ac}}$, $M_{\rho_{ac}}$ and M_S induced by the measurable families $\{Q_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$, $\{\rho_{ac}(\zeta)\}_{\zeta \in \mathbb{T}}$ and $\{S(\zeta)\}_{\zeta \in \mathbb{T}}$, respectively.

Using the spectral representation $\Pi(H_0^{ac}) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda)), M, \Phi'\}$ of Appendix C one gets that Q_{ac}, ρ_{ac} and S are presented in $\Pi(H_0^{ac})$ by multiplication operators $M_{Q'_{ac}}$, $M_{\rho'_{ac}}$ and $M_{S'}$ induced by the measurable families $\{Q'_{ac}(\lambda)\}_{\lambda \in \mathbb{R}}$, $\{\rho'_{ac}(\lambda)\}_{\lambda \in \mathbb{R}}$ and $\{S'(\lambda)\}_{\lambda \in \mathbb{R}}$, respectively. Notice that both families are related by

$$\begin{aligned}
Q'_{ac}(\lambda) &= Q_{ac}(e^{2i\arctan(\lambda)}), \quad \lambda \in \mathbb{R}, \\
\rho'_{ac}(\lambda) &= \rho_{ac}(e^{2i\arctan(\lambda)}), \quad \lambda \in \mathbb{R}, \\
S'(\lambda) &= S(e^{2i\arctan(\lambda)}), \quad \lambda \in \mathbb{R}.
\end{aligned}$$

Taking into account Theorem 3.7 we get

$$-\frac{1}{2}\mathrm{tr}(\Omega_-\rho U_0^*\Omega_-^*[V,Q])) = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left(\rho_{ac}'(\lambda)(Q_{ac}'(\lambda) - S'(\lambda)^*Q_{ac}'(\lambda)S'(\lambda))\right)\frac{d\lambda}{1+\lambda^2}. \tag{46}$$

Finally, replacing ρ by $(I + H_0^2)\rho$ we obtain (44) from (46). $\qquad\square$

Corollary 3.10. *If the assumptions of Theorem 3.9 are satisfied, then*

$$J' = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{tr}\left((\rho_{ac}'(\lambda) - S'(\lambda)\rho_{ac}'(\lambda)S'(\lambda)^*)\,Q_{ac}'(\lambda)\right)d\lambda.$$

Further, let $\phi : \mathbb{R} \longrightarrow [0,\infty)$ be Borel measurable and bounded. If $(1 + \lambda^2)\phi(\lambda)$, $\lambda \in \mathbb{R}$, is bounded and $\rho' = \phi(H_0)$, then $J' = 0$.

The proof of Corollary 3.10 follows from Corollary 3.8.

The charge Q was defined as a bounded self-adjoint operator. However, this definition is usually not sufficient in applications, cf. below. In [1, Definition 3.3] the notion of tempered charge was introduced. An unbounded self-adjoint operator Q is called a tempered charge if Q commutes with H_0 and for any bounded Borel set Λ of $\mathbb{R}$ the truncated charge $Q_\Lambda := QE_0(\Lambda)$ is bounded where $E_0(\cdot)$ is the spectral measure of H_0. For tempered charges we set

$$J_\Lambda' := -i\mathrm{tr}(W_-(I + H_0^2)\rho W_-^*(H - i)^{-1}[H, Q_\Lambda](H + i)^{-1}), \quad Q_\Lambda := QE_0(\Lambda).$$

Since $[Q, H_0] = 0$, we can decompose $Q' = Q_{ac} \oplus Q_s$. Let $\Pi(H_0^{ac}) = \{L^2(\mathbb{T}, d\lambda, \mathfrak{h}'(\lambda)), M', \Phi'\}$ be a spectral representation of H_0^{ac}. Then there is a measurable family $\{Q_{ac}'(\lambda)\}_{\lambda\in\mathbb{R}}$ of bounded operators such that Q_{ac} is unitarily equivalent to the multiplication operator $M_{Q_{ac}'}$ where

$$\begin{aligned}(M_{Q_{ac}'}\,\widehat{f'})(\lambda) &:= Q_{ac}'(\lambda)\,\widehat{f'}(\lambda), \quad \widehat{f'} \in \mathrm{dom}(M_{Q_{ac}'}), \quad \lambda \in \mathbb{R},\\ \mathrm{dom}(M_{Q_{ac}'}) &:= \{\widehat{f'} \in L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda) : Q_{ac}'(\lambda)\,\widehat{f'}(\lambda) \in L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda)\}.\end{aligned}$$

Obviously, one gets $Q_{\Lambda,ac}'(\lambda) = Q_{ac}'(\lambda)\chi_\Lambda(\lambda)$, $\lambda \in \mathbb{R}$. If Q is a tempered charge, then Q_{ac} is a tempered charge for H_0^{ac}, that is $\|Q_{ac}E_0^{ac}(\Lambda)\|_{\mathfrak{H}} < \infty$. Therefore, for a tempered charge one has

$$\sup_{\Lambda\in\mathcal{B}_b(\mathbb{R})}\mathrm{ess\text{-}sup}_{\lambda\in\Lambda}\|Q_{ac}'(\lambda)\|_{\mathfrak{h}'(\lambda)} < \infty \tag{47}$$

where ess-sup means the essential spectrum with respect to the Lebesgue measure on $\mathbb{R}$. In the following we denote the set of all bounded Borel sets of $\mathbb{R}$ by $\mathcal{B}_b(\mathbb{R})$.

Corollary 3.11. *Let $\mathcal{S}' = \{H, H_0\}$ be a $\mathfrak{L}_1$-scattering system. Further, let Q be a tempered charge and let ρ be a density operator. If*

$$\sup_{\Lambda\in\mathcal{B}_b(\mathbb{R})}\|QE_0(\Lambda)\|_{\mathfrak{H}}\|(I + H_0^2)\rho E_0(\Lambda)\|_{\mathfrak{H}} < \infty \tag{48}$$

then the limit $J' := \lim_{L\to\infty}J_{(-L,L)}'$ exists and the formula (44) is valid.

Proof. Applying Theorem 3.9 we find

$$J_\Lambda' = \frac{1}{2\pi}\int_\Lambda\mathrm{tr}(\rho_{ac}'(\lambda)(Q_{ac}'(\lambda) - S'(\lambda)^*Q_{ac}'(\lambda)S'(\lambda)))d\lambda, \quad \Lambda \in \mathcal{B}_b(\mathbb{R}).$$

From (48) which yields

$$\sup_{\Lambda\in\mathcal{B}_b(\mathbb{R})}\|Q_{ac}E_0(\Lambda)\|_{\mathfrak{H}}\|(I + H_0^2)\rho_{ac}E_0(\Lambda)\|_{\mathfrak{H}} < \infty$$

which yields

$$\|Q_{ac}E_0(\Lambda)\|_{\mathfrak{H}}\|(I + H_0^2)\rho_{ac}E_0(\Lambda)\|_{\mathfrak{H}} =$$
$$\mathrm{ess\text{-}sup}_{\lambda\in\Lambda}\|Q_{ac}'(\lambda)\|_{\mathfrak{h}'(\lambda)}\mathrm{ess\text{-}sup}_{\lambda\in\Lambda}(1 + \lambda^2)\|\rho_{ac}'(\lambda)\|_{\mathfrak{h}'(\lambda)}.$$

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Hence

$$\sup_{\Lambda\in\mathcal{B}_b(\mathbb{R})}\|Q_{ac}E_0(\Lambda)\|_{\mathfrak{H}}\|(I+H_0^2)\rho_{ac}E_0(\Lambda)\|_{\mathfrak{H}}=$$
$$\sup_{\Lambda\in\mathcal{B}_b(\mathbb{R})}\left\{\text{ess-sup}_{\lambda\in\Lambda}\|Q'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\text{ess-sup}_{\lambda\in\Lambda}(1+\lambda^2)\|\rho'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\right\}.$$

This gives

$$\sup_{\Lambda\in\mathcal{B}_b(\mathbb{R})}\text{ess-sup}_{\lambda\in\Lambda}\left\{(1+\lambda^2)\|Q'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\|\rho'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\right\}<\infty.$$

In particular, we have

$$\sup_{L>0}\text{ess-sup}_{\lambda\in(-L,L)}\left\{(1+\lambda^2)\|Q'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\|\rho'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\right\}<\infty. \tag{49}$$

Using the definition $T'(\lambda):=\frac{1}{2\pi}(I_{\mathfrak{h}'(\lambda)}-S'(\lambda))$, $\lambda\in\mathbb{R}$, we find the relation $T'(\lambda)=T(e^{2i\arctan(\lambda)})$ for a.e. $\lambda\in\mathbb{R}$. Taking into account (109) we get the estimate

$$\int_{\mathbb{R}}\|T'(\lambda)\|_{\mathfrak{L}_1}\frac{d\lambda}{1+\lambda^2}\le 2\|(H+i)^{-1}-(H_0+i)^{-1}\|_{\mathfrak{L}_1}. \tag{50}$$

Since

$$Q'_{ac}(\lambda)-S'(\lambda)Q'_{ac}S'(\lambda)=$$
$$2\pi i\left\{T'(\lambda)Q'_{ac}(\lambda)+Q_{ac}(\lambda)T'(\lambda)-2\pi iT'(\lambda)Q_{ac}(\lambda)T'(\lambda)\right\}$$

for a.e. $\lambda\in\mathbb{R}$ we find

$$\|\rho'_{ac}(\lambda)(Q'_{ac}(\lambda)-S'(\lambda)Q'_{ac}S'(\lambda))\|_{\mathfrak{L}_1}\le$$
$$\left(2+\tfrac{1}{\pi}\right)\|\rho'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\|Q'_{ac}(\lambda)\|_{\mathfrak{h}'(\lambda)}\|T'(\lambda)\|_{\mathfrak{L}_1}$$

for a.e. $\lambda\in\mathbb{T}$ where we have used that $\|T'(\lambda)\|_{\mathfrak{h}'(\lambda)}\le\frac{1}{\pi}$. Using (49) and (50) we verify that the integral

$$J'_{\mathbb{R}}:=\int_{\mathbb{R}}\text{tr}(\rho'_{ac}(\lambda)(Q'_{ac}(\lambda)-S'(\lambda)^*Q'_{ac}(\lambda)S'(\lambda)))d\lambda$$

exists and is finite. Hence

$$\lim_{L\to\infty}J'_{(-L,L)}=\lim_{L\to\infty}\frac{1}{2\pi}\int_{-L}^{L}\text{tr}(\rho'_{ac}(\lambda)(Q'_{ac}(\lambda)-S'(\lambda)^*Q'_{ac}(\lambda)S'(\lambda)))d\lambda=J'_{\mathbb{R}}$$

which completes the proof. $\qquad\square$

4 Examples

Let us consider examples where it is important that the Hamiltonian is not semibounded from below.

4.1 Landauer-Büttiker formula for dissipative operators

We consider the Schrödinger-type operator K in the Hilbert space $\mathfrak{K}=L^2((a,b))$ defined by

$$\text{dom}(K):=\left\{g\in W^{1,2}((a,b)):\begin{array}{l}\frac{1}{m(x)}g'(x)\in W^{1,2}((a,b))\\\left(\frac{1}{2m}g'\right)(a)=-\kappa_a g(a)\\\left(\frac{1}{2m}g'\right)(b)=\kappa_b g(b)\end{array}\right\}$$

and
$$(Kg)(x) = l(g)(x), \quad g \in \mathrm{dom}(K),$$

where
$$l(g)(x) = -\frac{d}{dx}\frac{1}{2m(x)}\frac{d}{dx}g(x) + V(x)g(x), \quad x \in (a, b),$$

$V \in L^\infty((a,b))$ and $m(x) > 0$ is real function such that $m \in L^\infty((a,b))$ and $\frac{1}{m} \in L^\infty((a,b))$. Furthermore, we assume $\kappa_a, \kappa_b \in \mathbb{C}_+ = \{z \in \mathbb{C} : \Im m(z) > 0\}$. The operator K is maximal dissipative and completely non-self-adjoint. Its spectrum consists of non-real isolated eigenvalues in $\mathbb{C}_-$ which accumulate at infinity.

To analyze the operator K it is useful to introduce the elementary solutions $v_a(x, z)$ and $v_b(x, z)$,

$$l(v_a(x, z)) - zv_a(x, z) = 0, \quad v_a(a, z) = 1, \quad \frac{1}{2m(a)}v'_a(a, z) = -\kappa_a, \tag{51}$$

$$l(v_b(x, z)) - zv_b(x, z) = 0, \quad v_b(b, z) = 1, \quad \frac{1}{2m(b)}v'_b(b, z) = \kappa_b, \tag{52}$$

$x \in [a, b]$, $z \in \mathbb{C}$, which always exist. The Wronskian of $v_a(x, z)$ and $v_b(x, z)$ is defined by $W(z)$, i.e.

$$W(z) = v_a(x, z)\frac{1}{2m(x)}v'_b(x, z) - v_b(x, z)\frac{1}{2m(x)}v'_a(x, z). \tag{53}$$

We note that the Wronskian does not depend on x. Obviously, the functions $v_{*a}(x, z)$ and $v_{*b}(x, z)$,

$$v_{*a}(x, z) := \overline{v_a(x, \overline{z})} \quad \text{and} \quad v_{*b}(x, z) := \overline{v_b(x, \overline{z})}, \quad z \in \mathbb{C}. \tag{54}$$

$x \in [a, b]$, $z \in \mathbb{C}$, are also elementary solutions of

$$l(v_{*a}(x, z)) - zv_{*a}(x, z) = 0, \quad v_{*a}(a, z) = 1, \quad \frac{1}{2m(a)}v'_{*a}(a, z) = -\overline{\kappa_a}, \tag{55}$$

$$l(v_{*b}(x, z)) - zv_{*b}(x, z) = 0, \quad v_{*b}(b, z) = 1, \quad \frac{1}{2m(b)}v'_{*b}(b, z) = \overline{\kappa_b}, \tag{56}$$

$x \in [a, b]$. The Wronskian of $v_{*a}(x, z)$ and $v_{*b}(x, z)$ is denoted by $W_*(z)$ and is also independent from x. Using the elementary solutions one gets the representation

$$((H - z)^{-1}f)(x) = \tag{57}$$
$$-\frac{v_b(x, z)}{W(z)}\int_a^x dy\, v_a(y, z)f(y) - \frac{v_a(x, z)}{W(z)}\int_x^b dy\, v_b(y, z)f(y),$$

for $z \in \varrho(H)$ and $f \in L^2([a, b])$ and

$$((H^* - z)^{-1}f)(x) = \tag{58}$$
$$-\frac{v_{*b}(x, z)}{W_*(z)}\int_a^x dy\, v_{*a}(y, z)f(y) - \frac{v_{*a}(x, z)}{W_*(z)}\int_x^b dy\, v_{*b}(y, z)f(y),$$

for $z \in \varrho(H^*)$ and $f \in L^2([a, b])$, see [13].

Since H is completely non-self-adjoint the maximal dissipative operator H can be completely characterized by its characteristic function $\theta_K(z)$, $z \in \varrho(H) \cap \varrho(H^*)$. The definition of the characteristic function relies on the so-called boundary operators $T(z) : \mathfrak{K} \longrightarrow \mathbb{C}^2$, $z \in \varrho(H)$ and $T_*(z) : \mathfrak{K} \longrightarrow \mathbb{C}^2$, $z \in \varrho(H^*)$, which are defined in [13]. Introducing representations

$$\kappa_a = q_a + \frac{i}{2}\alpha_a^2 \quad \text{and} \quad \kappa_b = q_b + \frac{i}{2}\alpha_b^2, \quad \alpha_a, \alpha_b > 0, \tag{59}$$

the boundary operators are defined by

$$T(z)f := \begin{pmatrix} \alpha_b((H - z)^{-1}f)(b) \\ -\alpha_a((H - z)^{-1})f(a) \end{pmatrix} \tag{60}$$

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and

$$T_*(z)f := \begin{pmatrix} \alpha_b((H^* - z)^{-1}f)(b) \\ -\alpha_a((H^* - z)^{-1}f)(a) \end{pmatrix}, \tag{61}$$

$f \in L^2([a,b])$. Using the resolvent representations (57) and (58) we obtain

$$T(z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\, v_a(y,z)f(y) \\ \alpha_a \int_a^b dy\, v_b(y,z)f(y) \end{pmatrix} \tag{62}$$

and

$$T_*(z)f = \frac{1}{W_*(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\, v_{*a}(y,z)f(y) \\ \alpha_b \int_a^b dy\, v_{*b}(y,z)f(y) \end{pmatrix}, \tag{63}$$

$f \in L^2([a,b])$. The adjoint operators are given by

$$
\begin{aligned}
(T(z)^*\xi)(x) &= \frac{1}{\overline{W(z)}}\left(-\alpha_b\overline{v_a(x,z)}, \alpha_a\overline{v_b(x,z)}\right)\xi \\
&= \frac{1}{W_*(\overline{z})}\left(-\alpha_b v_{*a}(x,\overline{z}), \alpha_a v_{*b}(x,\overline{z})\right)\xi,
\end{aligned}
\tag{64}
$$

and

$$
\begin{aligned}
(T_*(z)^*\xi)(x) &= \frac{1}{\overline{W_*(z)}}\left(-\alpha_b\overline{v_{*a}(x,z)}, \alpha_a\overline{v_{*b}(x,z)}\right)\xi \\
&= \frac{1}{W(\overline{z})}\left(-\alpha_b v_a(x,\overline{z}), \alpha_a v_b(x,\overline{z})\right)\xi,
\end{aligned}
\tag{65}
$$

where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^a \end{pmatrix} \in \mathbb{C}^2. \tag{66}$$

The characteristic function $\Theta_K(\cdot)$ of the maximal dissipative operator H is a two-by-two matrix-valued function which satisfies the relation

$$\Theta_K(z)T(z)f = T_*(z)f, \quad z \in \varrho(H) \cap \varrho(H^*), \quad \alpha_a, \alpha_b > 0, \tag{67}$$

$f \in L^2([a,b])$. It depends meromorphically on $z \in \varrho(H) \cap \varrho(H^*)$ and is contractive in $\mathbb{C}_-$, i.e.

$$\|\Theta_K(z)\| \le 1 \quad \text{for} \quad z \in \mathbb{C}_-. \tag{68}$$

Using the elementary solutions the characteristic function $\Theta_K(\cdot)$ takes the form

$$\Theta_K(z) = I_{\mathbb{C}^2} + i\frac{1}{W_*(z)}\begin{pmatrix} \alpha_b^2 v_{*a}(b,z) & -\alpha_b\alpha_a \\ -\alpha_b\alpha_a & \alpha_a^2 v_{*b}(a,z) \end{pmatrix}. \tag{69}$$

for $z \in \varrho(H) \cap \varrho(H^*)$, cf. [13]

Since the operator K is maximal dissipative there is a larger Hilbert space $\mathfrak{H}$ and a self-adjoint operator H such that $\mathfrak{K}$ is embed in $\mathfrak{H}$ and the relation

$$P_{\mathfrak{K}}^{\mathfrak{H}}(H - z)^{-1} \upharpoonright \mathfrak{K} = (K - z)^{-1}, \quad z \in \mathbb{C}_+,$$

is satisfied. The self-adjoint operator H is called a self-adjoint dilation of K. If the condition
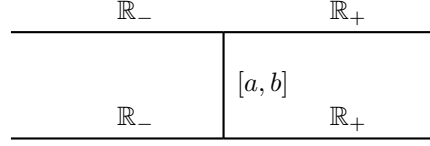
$$\operatorname{clospan}\{(H - z)^{-1}\mathfrak{K} : z \in \mathbb{C} \setminus \mathbb{R}\} = \mathfrak{H}$$

is satisfied, then H is called a minimal self-adjoint dilation K of H. Minimal self-adjoint dilations of maximal dissipative operators are determined up to a certain isomorphism, in particular, all minimal self-adjoint dilations are unitarily equivalent.

In the present case the minimal self-adjoint dilation of the maximal dissipative operator H can be constructed in an explicit manner. In accordance with [13] we introduce the larger Hilbert space

$$\mathfrak{H} = \mathfrak{D}_- \oplus \mathfrak{K} \oplus \mathfrak{D}_+ \tag{70}$$

where $\mathfrak{D}_\pm := L^2(\mathbb{R}_\pm, \mathbb{C}^2)$. Introducing the graph Ω,

$$
\begin{array}{ccc}
\underline{\quad\mathbb{R}_-\quad} & & \underline{\quad\mathbb{R}_+\quad} \\
& \left| \begin{array}{c} [a,b] \end{array} \right. & \\
\underline{\quad\mathbb{R}_-\quad} & & \underline{\quad\mathbb{R}_+\quad}
\end{array}
$$

one can write the Hilbert space $\mathfrak{H}$ as $L^2(\hat{\Omega})$. Further, we define

$$\vec{g} := g_- \oplus g \oplus g_+ \tag{71}$$

where

$$g_-(x) := \begin{pmatrix} g_-^b(x) \\ g_-^a(x) \end{pmatrix} \quad \text{and} \quad g_+(x) := \begin{pmatrix} g_+^b(x) \\ g_+^a(x) \end{pmatrix} \tag{72}$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively. Let us introduce the matrices $K_\pm^a$ and $K_\pm^b$ which are defined by

$$K_-^a := \begin{pmatrix} 0 & 0 \\ 1 & \kappa_a \end{pmatrix} \quad \text{and} \quad K_+^a := \begin{pmatrix} 0 & 0 \\ 1 & \overline{\kappa_a} \end{pmatrix} \tag{73}$$

as well as

$$K_-^b := \begin{pmatrix} 1 & -\kappa_b \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad K_+^b := \begin{pmatrix} 1 & -\overline{\kappa_b} \\ 0 & 0 \end{pmatrix}. \tag{74}$$

Further we set

$$\Lambda := \begin{pmatrix} \alpha_b & 0 \\ 0 & \alpha_b \end{pmatrix}$$

Using these notations the self-adjoint dilation K is defined by

$$\text{dom}(H) := \left\{ \vec{g} \in \mathfrak{H} : \begin{array}{l} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2), \\ g, \frac{1}{m}g' \in W^{1,2}([a,b]), \\ K_-^a g_a + K_-^b g_b = \Lambda g_-(0), \\ K_+^a g_a + K_+^b g_b = \Lambda g_+(0) \end{array} \right\} \tag{75}$$

and

$$H\vec{g} := -i\frac{d}{dx}g_- \oplus l(g) \oplus -i\frac{d}{dx}g_+, \qquad \vec{g} \in \text{dom}(H), \tag{76}$$

where,

$$g_a = \begin{pmatrix} \frac{1}{2m(a)}g'(a) \\ g(a) \end{pmatrix} \quad \text{and} \quad g_b = \begin{pmatrix} \frac{1}{2m(b)}g'(b) \\ g(b) \end{pmatrix}, \tag{77}$$

With respect to a graph picture the operator H looks like

$$\alpha_b g_-^b(0) = \frac{1}{2m(b)}g'(b) - \kappa_b g(b) \qquad\qquad \frac{1}{2m(b)}g'(b) - \overline{\kappa_b}g(b) = \alpha_b g_+^b(0)$$

$$\underline{\qquad\qquad\qquad\qquad}) \qquad\qquad\qquad (\underline{\qquad\qquad\qquad\qquad}$$

$$\qquad -i\frac{d}{dx}g_-^b \qquad\qquad\qquad\qquad\qquad -i\frac{d}{dx}g_+^b$$

$$\qquad\qquad\qquad\qquad\qquad\qquad l(g)$$

$$\qquad -i\frac{d}{dx}g_-^a \qquad\qquad\qquad\qquad\qquad -i\frac{d}{dx}g_+^a$$

$$\underline{\qquad\qquad\qquad\qquad}) \qquad\qquad\qquad (\underline{\qquad\qquad\qquad\qquad}$$

$$\alpha_a g_-^a(0) = \frac{1}{2m(a)}g'(a) + \kappa_a g(a) \qquad \frac{1}{2m(a)}g'(a) + \overline{\kappa_a}g(a) = \alpha_a g_+^a(0)$$

We define another self-adjoint operator H_0 by setting $\alpha_b = \alpha_a = 0$. In this case we get

$$\operatorname{dom}(H_0) := \left\{ \vec{g} \in \mathfrak{H} : \begin{array}{c} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2), \\ g, \frac{1}{m}g' \in W^{1,2}((a,b)), \\ K_-^a g_a + K_-^b g_b = 0, \\ K_+^a g_a + K_+^b g_b = 0, \\ g_-(0) = g_+(0) \end{array} \right\}$$

and

$$H_0 \vec{g} := -i\frac{d}{dx}g_- \oplus l(g) \oplus -i\frac{d}{dx}g_+, \qquad \vec{g} \in \operatorname{dom}(H_0),$$

Setting $\mathfrak{D} = \mathfrak{D}_- \oplus \mathfrak{D}_+ = L^2(\mathbb{R}, \mathbb{C}^2)$ we obtain

$$\mathfrak{H} = \mathfrak{D} \oplus \mathfrak{K}$$

and

$$H_0 = T \oplus K_0$$

where T is the momentum operator given by $\operatorname{dom}(T) := W^{1,2}(\mathbb{R}, \mathbb{C}^2)$

$$(Tf)(x) := -i\frac{d}{dx}f(x), \quad f \in \operatorname{dom}(T),$$

and K_0 is defined by

$$\operatorname{dom}(K_0) := \left\{ \vec{g} \in \mathfrak{H} : \begin{array}{c} \frac{1}{m}g' \in W^{1,2}((a,b)) \\ (\frac{1}{2m}g)(b) = q_b g(b) \\ (\frac{1}{2m}g)(a) = -q_a g(a) \end{array} \right\}$$

Since the operator K_0 is discrete one gets $H_0^{ac} = T$ and $\mathfrak{H}^{ac}(H_0) = L^2(\mathbb{R}, \mathbb{C}^2)$. One easily checks that the resolvent difference is a trace class operator. This is due to the fact that both operators H and H_0 are self-adjoint extensions of the symmetric operator $\widetilde{H}$,

$$\operatorname{dom}(\widetilde{H}) := \left\{ \vec{g} \in \mathfrak{H} : \begin{array}{c} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2) \\ g, \frac{1}{m}g' \in W^{1,2}((a,b)) \\ g_a = g_b = 0 \\ g_\pm(0) = 0 \end{array} \right\},$$

which has finite deficiency indices. Hence $\mathcal{S} = \{H, H_0\}$ is trace class scattering system. In particular, the wave operators $W_\pm(H, H_0)$ exist and are complete.

One easily checks that $\Pi(H_0^{ac}) = \{L^2(\mathbb{R}, d\lambda, \mathbb{C}^2), M, \mathcal{F}\}$ where M is the multiplication operator induced by the independent variable λ and $\mathcal{F}$ denotes the Fourier transform

$$(\mathcal{F}f)(\lambda) = \frac{1}{2\pi}\int_\mathbb{R} e^{-i\lambda x}f(x)dx, \qquad f \in L^2(\mathbb{R}, dx, \mathbb{C}^2).$$

It is known that the scattering operator $S(H, H_0) = W_+(H, H_0)^* W_-(H, H_0)$ is unitarily equivalent to the multiplication operator M_{Θ^*} induced by the measurable family $\{\Theta(\lambda)^*\}_{\lambda \in \mathbb{R}}$ in $L^2(\mathbb{R}, d\lambda, \mathbb{C}^2)$ where

$$\Theta(\lambda) = \lim_{\eta \to +0} \Theta(\lambda - i\eta) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\frac{1}{W_*(\lambda)} \begin{pmatrix} \alpha_b^2 v_{*a}(b, \lambda) & -\alpha_b \alpha_a \\ -\alpha_b \alpha_a & \alpha_a^2 v_{*b}(a, \lambda) \end{pmatrix}$$

which exist and is contractive for $\lambda \in \mathbb{R}$. Setting

$$\theta_b(\lambda) := W(\lambda) - i\alpha_b^2 v_a(b, \lambda) \quad \text{and} \quad \theta_a(\lambda) := W(\lambda) - i\alpha_a^2 v_b(a, \lambda),$$

$\lambda \in \mathbb{R}$, we find the representation

$$\Theta(\lambda) = \frac{1}{\overline{W(\lambda)}} \begin{pmatrix} \overline{\theta_b(\lambda)} & -i\alpha_b\alpha_a \\ -i\alpha_b\alpha_a & \overline{\theta_a(\lambda)} \end{pmatrix}$$

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and

$$\Theta(\lambda)^* = \frac{1}{W(\lambda)} \begin{pmatrix} \theta_b(\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & \theta_a(\lambda) \end{pmatrix}. \tag{78}$$

Since $\Theta(\lambda)^*\Theta(\lambda) = I_{\mathbb{C}^2}$ for $\lambda \in \mathbb{R}$ we obtain

$$1 = |\theta_b(\lambda)|^2 + \alpha_b^2\alpha_a^2 = |\theta_a(\lambda)|^2 + \alpha_b^2\alpha_a^2 \quad \text{and} \quad \theta_a(\lambda) = \overline{\theta_b(\lambda)} \tag{79}$$

for $\lambda \in \mathbb{R}$.

Let ρ be a steady state for H_0. Obviously, the steady state is unitarily equivalent to the multiplication M_ρ induced by a measurable family $\{\rho(\lambda)\}_{\lambda \in \mathbb{R}}$ of non-negative bounded self-adjoint operators acting in $\mathbb{C}^2$. We use the representation

$$\rho(\lambda) = \begin{pmatrix} \rho_b(\lambda) & \overline{\tau(\lambda)} \\ \tau(\lambda) & \rho_a(\lambda) \end{pmatrix} \geq 0, \quad \lambda \in \mathbb{R}. \tag{80}$$

Notice that $\rho(\lambda) \geq 0$ if and only if the conditions $\rho_b(\lambda) \geq 0$, $\rho_a(\lambda) \geq 0$ and

$$|\tau(\lambda)|^2 \leq \rho_b(\lambda)\rho_a(\lambda)$$

is satisfied for a.e. $\lambda \in \mathbb{R}$. Moreover, ρ and $(I + H_0^2)\rho$ are bounded operators if and only the conditions

$$\text{ess-sup}_{\lambda \in \mathbb{R}} \{\rho_b(\lambda) + \rho_a(\lambda) + |\tau(\lambda)|\} < \infty.$$

and

$$\text{ess-sup}_{\lambda \in \mathbb{R}}(1 + \lambda^2) \{\rho_b(\lambda) + \rho_a(\lambda) + |\tau(\lambda)|\} < \infty. \tag{81}$$

are satisfied, respectively.

In [14] the current related to the self-adjoint operator H was calculated in accordance with [19]. To this end the generalized incoming eigenfunctions $\psi(x, \lambda, a)$ and $\psi(x, \lambda, b)$, $x \in \Omega$, $\gamma \in \{a, b\}$, $\lambda \in \mathbb{R}$ of H were computed and the current $j_\rho(x, \lambda)$ was defined by

$$j_\rho(x, \lambda) := \mu_b(\lambda)\Im m \left(\frac{1}{m(x)} \overline{\psi(x, \lambda, b)} m(x)\psi'(x, \lambda, b) \right) +$$
$$\mu_a(\lambda)\Im m \left(\frac{1}{m(x)} \overline{\psi(x, \lambda, a)} m(x)\psi'(x, \lambda, a) \right)$$

for $x \in \Omega$, $\lambda \in \mathbb{R}$, where $\mu_b(\lambda)$ and $\mu_a(\lambda)$ are the eigenvalues of $\rho(\lambda)$. It turns out that $j_\rho(x, \lambda)$ is independent from x, that is $j_\rho(\lambda) := j_\rho(x, \lambda)$, and admits the representation

$$j_\rho(\lambda) = \text{tr}(\rho(\lambda)C(\lambda)), \quad \lambda \in \mathbb{R}$$

where

$$C(\lambda) := -\frac{1}{2\pi i} \frac{\alpha_b\alpha_a}{W(\lambda)} E\Theta(\lambda)^*, \quad \lambda \in \mathbb{R},$$

and

$$E := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

cf. Proposition 4.1 of [14]. If $\text{tr}(\rho(\lambda)) \in L^1(\mathbb{R}, d\lambda)$, then the full current j_ρ is given by

$$j_\rho = \int_{\mathbb{R}} j_\rho(\lambda)d\lambda$$

cf. Proposition 4.1 of [14]. Using (78) and (80) we find

$$j_\rho = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{-\alpha_b^2\alpha_a^2(\rho_b(\lambda) - \rho_a(\lambda)) + i\alpha_b\alpha_b(\tau(\lambda)\theta_a(\lambda) - \overline{\tau(\lambda)}\theta_b(\lambda))}{|W(\lambda)|^2} d\lambda. \tag{82}$$

Let us calculate the current in accordance with Theorem 3.9. To define charges we note that $\mathfrak{D}$ admits the decomposition

$$\mathfrak{D} = \begin{array}{c} \mathfrak{D}_b \\ \oplus \\ \mathfrak{D}_a \end{array}.$$

By Q_b and Q_a we denote the projections form $\mathfrak{D}$ onto $\mathfrak{D}_b$ and $\mathfrak{D}_a$, respectively. The operators Q_b and Q_a commute with H_0 and can be regarded as charges. The charge matrices are given

$$Q_b(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad Q_a(\lambda) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \lambda \in \mathbb{R}.$$

Applying Theorem 3.9 we find

$$J^{\mathcal{S}}_{\rho,Q_a} = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{tr}\left(\rho(\lambda)\left(Q_a(\lambda) - \Theta(\lambda)Q_a(\lambda)\Theta(\lambda)^*\right)\right) d\lambda.$$

A straightforward computation shows that

$$Q_a(\lambda) - \Theta(\lambda)Q_a(\lambda)\Theta(\lambda)^* = \frac{1}{|W(\lambda)|^2} \begin{pmatrix} -\alpha_b^2\alpha_a^2 & i\alpha_b\alpha_a\theta_a(\lambda) \\ -i\alpha_b\alpha_a\overline{\theta_a(\lambda)} & \alpha_b^2\alpha_a^2 \end{pmatrix}.$$

Taking into account (80) we obtain

$$\mathrm{tr}(\rho(\lambda)(Q_a(\lambda) - \Theta(\lambda)Q_a(\lambda)\Theta(\lambda)^*)) =$$
$$\frac{1}{|W(\lambda)|^2}\left(-\alpha_b^2\alpha_a^2(\rho_b(\lambda) - \rho_a(\lambda)) + i\alpha_a\alpha_b(\tau(\lambda)\theta_a(\lambda) - \overline{\tau(\lambda)}\,\overline{\theta_a(\lambda)})\right)$$

which yields

$$J^{\mathcal{S}}_{\rho,Q_a} = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{-\alpha_b^2\alpha_a^2(\rho_b(\lambda) - \rho_a(\lambda)) + i\alpha_a\alpha_b(\tau(\lambda)\theta_a(\lambda) - \overline{\tau(\lambda)}\,\overline{\theta_a(\lambda)})}{|W(\lambda)|^2} \, d\lambda.$$

Using (79) we immediately get from (82) that $J^{\mathcal{S}}_{\rho,Q_a} = j_\rho$. Comparing with [14] the proof is much shorter. Moreover, from Proposition 4.1 of [14] we get that

$$|J^{\mathcal{S}}_{\rho,Q_a}| \leq \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{tr}(\rho(\lambda)) \, d\lambda = \frac{1}{2\pi} \int_{\mathbb{R}} (\rho_b(\lambda) + \rho_a(\lambda)) \, d\lambda$$

By (81) the last integral exists.

4.2 Landauer-Büttiker formula for a pseudo-relativistic system

We consider the Hilbert space $L^2(\mathbb{R}, \mathbb{C}^2)$ and the symmetric Dirac operator

$$(A\vec{f})(x) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{d}{dx}\vec{f}(x) + \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} \vec{f}(x), \quad \vec{f} \in \mathrm{dom}(A), \ x \in \mathbb{R},$$

where $a > 0$ and

$$\mathrm{dom}(A) := \{\vec{f} \in W^{1,2}(\mathbb{R}, \mathbb{C}^2) : \vec{f}(0) = 0\}$$

and

$$\vec{f} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \quad f_1, f_2 \in L^2(\mathbb{R}, dx).$$

The deficiency indices $n_\pm(A)$ are equal two. The operator A is completely non-self-adjoint. The domain of the adjoint operator is given by

$$\mathrm{dom}(A^*) = W^{1,2}(\mathbb{R}_-, \mathbb{C}^2) \oplus W^{1,2}(\mathbb{R}_+, \mathbb{C}^2).$$

Its Weyl function $M(z)$ was calculated in [5]. One has

$$M(z) = \begin{pmatrix} i\frac{\sqrt{z+a}}{\sqrt{z-a}} & 0 \\ 0 & i\frac{\sqrt{z-a}}{\sqrt{z+a}} \end{pmatrix}, \qquad z \in \mathbb{C}_+,$$

where the cut of the square root $\sqrt{\cdot}$ is fixed along the non-negative real axis. We define a self-adjoint extension H_0 of A by $H_0 = A^* \upharpoonright \operatorname{dom}(H_0)$,

$$\operatorname{dom}(H_0) = \{\vec{f} \in \operatorname{dom}(A^*) : f_2(-0) = 0, \quad f_1(+0) = 0\}.$$

The operator H_0 is self-adjoint and absolutely continuous. Its spectrum is given by $\sigma(H_0) = \sigma_{ac}(H_0) = \mathbb{R} \setminus (-a, a)$. It is not hard to see that the H_0 has the form

$$H_0 = H_- \oplus H_+$$

where $H_\pm$ are are self-adjoint operators in $L^2(\mathbb{R}_\pm, \mathbb{C}^2)$, respectively. A straightforward computation shows that the operator H_- and H_+ are unitarily equivalent to the operator K_-,

$$(K_- f)(x) \quad := \quad i\frac{d}{dx}f(x) - af(-x), \quad f \in \operatorname{dom}(K_-), \tag{83}$$

$$\operatorname{dom}(K_-) \quad := \quad \{W^{1,2}(\mathbb{R}_-) \oplus W^{1,2}(\mathbb{R}_+) : f(-0) = -f(+0)\}, \tag{84}$$

and K_+,

$$(K_+ f)(x) := i\frac{d}{dx}f(x) - af(-x), \quad f \in \operatorname{dom}(K_+) := W^{1,2}(\mathbb{R}),$$

defined in $L^2(\mathbb{R})$, respectively.

The limit $M(\lambda) := \lim_{y \to +0} M(\lambda + iy)$ exist for every point $\lambda \in \mathbb{R} \setminus \{-a, a\}$. One has

$$M(\lambda) = \begin{pmatrix} i\frac{\sqrt{\lambda+a}}{\sqrt{\lambda-a}} & 0 \\ 0 & i\frac{\sqrt{\lambda-a}}{\sqrt{\lambda+a}} \end{pmatrix}, \quad \lambda \in \mathbb{R} \setminus \{-a, a\}.$$

Hence

$$\Im m(M(\lambda)) = \begin{pmatrix} \sqrt{\frac{\lambda+a}{\lambda-a}} & 0 \\ 0 & \sqrt{\frac{\lambda-a}{\lambda+a}} \end{pmatrix}, \quad \lambda \in \mathbb{R} \setminus [-a, a],$$

and $\Im m(M(\lambda)) = 0$ for $\lambda \in (-a, a)$. We set $\mathfrak{h}(\lambda) := \operatorname{ran}(\Im m(M(\lambda)))$, $\lambda \in \mathbb{R} \setminus \{-a, a\}$. Obviously, we get

$$\mathfrak{h}(\lambda) = \begin{cases} \mathbb{C}^2 & \lambda \in \mathbb{R} \setminus [-a, a] \\ 0 & \lambda \in (-a, a). \end{cases}$$

We consider the direct integral $L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda))$. I turns out that there is an isometry Φ acting from $\mathfrak{H}$ onto $L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda))$ such that the triplet $\Pi(H_0) = \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}(\lambda)), \mathcal{M}, \Phi\}$ is a spectral representation of H_0.

Another self-adjoint extension H of A is defined by choosing a self-adjoint operator B,

$$B = \begin{pmatrix} b_- & \overline{r} \\ r & b_+ \end{pmatrix}, \quad b_-, b_+ \in \mathbb{R}, \quad r \in \mathbb{C},$$

acting on $\mathbb{C}^2$ and setting

$$\operatorname{dom}(H) := \left\{ \vec{f} \in \operatorname{dom}(A^*) : \begin{array}{ccc} f_1(-0) & = & b_- f_2(-0) + \overline{r} f_1(+0) \\ f_2(+0) & = & r f_2(-0) + b_+ f_1(+0) \end{array} \right\}$$

The self-adjoint extension H can be regarded as the Hamiltonian of some point interaction at zero. Since the deficiency indices of A are finite the resolvent difference of H and H_0 is trace class operator.

We consider the trace class scattering system $\mathcal{S} = \{H, H_0\}$. Following [2] the scattering matrix $\{S(\lambda)\}_{\lambda \in \mathbb{R}}$ admits the representation

$$S(\lambda) = I_{\mathfrak{h}(\lambda)} + 2i\sqrt{\Im m(M(\lambda))}(B - M(\lambda))^{-1}\sqrt{\Im m(M(\lambda))},$$

$\lambda \in \mathbb{R} \setminus [-a, a]$. We find

$$(B - M(\lambda))^{-1} = \frac{1}{\det(B - M(\lambda))} \begin{pmatrix} b_+ - i\frac{\sqrt{\lambda - a}}{\sqrt{\lambda + a}} & -\overline{r} \\ -r & b_- - i\frac{\sqrt{\lambda + a}}{\sqrt{\lambda - a}} \end{pmatrix}$$

for $\lambda \in \mathbb{R} \setminus [-a, a]$. The transition matrix $\{T(\lambda)\}_{\lambda \in \mathbb{R}}$ is defined $T(\lambda) := S(\lambda) - I_{\mathfrak{h}(\lambda)}$, $\lambda \in \mathbb{R} \setminus [-a, a]$, which yields

$$T(\lambda) = 2i\sqrt{\Im m(M(\lambda))}(B - M(\lambda))^{-1}\sqrt{\Im m(M(\lambda))}, \quad \lambda \in \mathbb{R} \setminus [-a, a].$$

Using the representation

$$T(\lambda) = \begin{pmatrix} t_{--}(\lambda) & t_{-+}(\lambda) \\ t_{+-}(\lambda) & t_{++}(\lambda) \end{pmatrix}$$

we find

$$
\begin{aligned}
t_{--}(\lambda) &= \frac{2i}{\det(B - M(\lambda))}\left(b_+ \frac{\sqrt{\lambda + a}}{\sqrt{\lambda - a}} - i\right) \\
t_{-+}(\lambda) &= -\overline{r}\frac{2i}{\det(B - M(\lambda))} \\
t_{+-}(\lambda) &= -r\frac{2i}{\det(B - M(\lambda))} \\
t_{++}(\lambda) &= \frac{2i}{\det(B - M(\lambda))}\left(b_- \frac{\sqrt{\lambda - a}}{\sqrt{\lambda + a}} - i\right)
\end{aligned}
$$

We set

$$\sigma(\lambda) := |t_{-+}(\lambda)|^2 = |t_{+-}(\lambda)|^2 = \frac{4|r|^2}{|\det(B - M(\lambda))|^2}, \quad \lambda \in \mathbb{R} \setminus [-a, a],$$

which is the cross section between the left- and right-hand scattering channels. Since $\|T(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} \leq 2$, $\lambda \in \mathbb{R} \setminus [-a, a]$, we find $\sigma(\lambda) \leq 2$, $\lambda \in \mathbb{R} \setminus [-a, a]$, which yields

$$\frac{2|r|^2}{|\det(B - M(\lambda))|^2} \leq 1, \quad \lambda \in \mathbb{R} \setminus [-a, a].$$

Let $Q_\pm$ be the orthogonal projection from $L^2(\mathbb{R}, \mathbb{C}^2)$ onto $L^2(\mathbb{R}_\pm, \mathbb{C}^2)$. Obviously, $Q_\pm$ commute with H_0. With respect to the spectral representation the charges $Q_\pm$ correspond to

$$Q_-(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad Q_+(\lambda) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \lambda \in \mathbb{R} \setminus [-a, a].$$

If the steady state ρ is chosen as

$$\rho = \rho_- \oplus \rho_+,$$

then the corresponding charge matrices are given by

$$\rho(\lambda) = \begin{pmatrix} \rho_-(\lambda) & 0 \\ 0 & \rho_+(\lambda) \end{pmatrix}, \quad \lambda \in \mathbb{R} \setminus [-a, a].$$

where $\rho_\pm(\lambda)$ are non-negative bounded Borel functions on $\mathbb{R} \setminus [-a, a]$. The operator $(I + H_0^2)\rho$ is bounded if and only if ess-sup$_{\lambda \in \mathbb{R} \setminus [-a, a]}(1 + \lambda^2)\rho_\pm(\lambda) < \infty$. Applying Theorem 3.9 we find that the current $J^{\mathcal{S}}_{\rho, Q_-}(|r|)$ is given by

$$
\begin{aligned}
J^{\mathcal{S}}_{\rho, Q_-}(|r|) &= \frac{1}{2\pi} \int_{\mathbb{R} \setminus [-a, a]} (\rho_-(\lambda) - \rho_+(\lambda))\sigma(\lambda)d\lambda \\
&= \frac{2|r|^2}{\pi} \int_{\mathbb{R} \setminus [-a, a]} \frac{\rho_-(\lambda) - \rho_+(\lambda)}{|\det(B - M(\lambda))|^2}d\lambda
\end{aligned}
$$

A very simple case arises if we set $b_\pm = 0$. In this case we have

$$J^{\mathcal{S}}_{\rho, Q_-}(|r|) = \frac{2|r|^2}{(1 + |r|^2)^2 \pi} \int_{\mathbb{R} \setminus [-a, a]} (\rho_-(\lambda) - \rho_+(\lambda)) d\lambda.$$

The magnitude of the current becomes maximal in this case if $|r| = 1$, that is, if

$$J^{\mathcal{S}}_{\rho, Q_-}(1) = \frac{1}{2\pi} \int_{\mathbb{R} \setminus [-a, a]} (\rho_-(\lambda) - \rho_+(\lambda)) d\lambda.$$

Since $\sigma(\lambda) \leq 2$ we find the estimate

$$|J^{\mathcal{S}}_{\rho, Q_-}(|r|)| \leq \frac{1}{\pi} \int_{\mathbb{R} \setminus [-a, a]} (\rho_+(\lambda) + \rho_-(\lambda)) d\lambda.$$

Obviously $J^{\mathcal{S}}_{\rho, Q_-}(0) = 0$ which is natural. In this case the self-adjoint operator H decomposes into a left and right hand side extension which have nothing to do with each other. However, one also has $\lim_{|r| \to \infty} J^{\mathcal{S}}_{\rho, Q_-}(|r|) = 0$.

For electrons one has to choose

$$\rho_\pm(\lambda) := \rho_{FD}(\lambda - \mu_\pm), \quad \lambda \in \mathbb{R},$$

where $\mu_\pm$ is the so-called Fermi energy and $\rho_{FD}(\lambda)$ is the Fermi-Dirac distribution

$$\rho_{FD}(\lambda) = (1 + e^{\beta \lambda})^{-1}, \quad \lambda \in \mathbb{R}, \quad \beta > 0.$$

Obviously, the condition ess-sup$_{\mathbb{R} \setminus [-a, a]}(1 + \lambda^2) \rho_\pm(\lambda) < \infty$ is not satisfied. However, it turns out that

$$\rho_-(\lambda) - \rho_+(\lambda) = e^{\beta \lambda}(e^{-\beta \mu_+} - e^{-\beta \mu_-}) \rho_-(\lambda) \rho_+(\lambda), \quad \lambda \in \mathbb{R}.$$

satisfies ess-sup$_{\mathbb{R} \setminus [-a, a]}(1 + \lambda^2)|\rho_-(\lambda) - \rho_+(\lambda)| < \infty$ which shows that the current $J^{\mathcal{S}}_{\rho, Q_-}$ is well defined.

Appendix: Spectral representations

A Spectral representation for unitary operators

Let $\mathfrak{k}$ be a separable Hilbert space and let μ a Borel measure on the unit circle $\mathbb{T}$. We consider the Hilbert space $L^2(\mathbb{T}, d\mu, \mathfrak{k})$ and the multiplication operator $\mathcal{Z}$ defined by

$$(\mathcal{Z} \widehat{f})(\zeta) = \zeta \widehat{f}(\zeta), \quad \widehat{f} \in L^2(\mathbb{T}, d\mu, \mathfrak{k}).$$

Let $\{P(\zeta)\}_{\zeta \in \mathbb{T}}$ be a measurable family of orthogonal projections in $\mathfrak{k}$. Setting

$$(P \widehat{f})(\zeta) = P(\zeta) \widehat{f}(\zeta), \quad \widehat{f} \in L^2(\mathbb{T}, d\mu, \mathfrak{k}), \tag{85}$$

one defines orthogonal projection on $L^2(\mathbb{T}, d\mu, \mathfrak{k})$. The subspace $PL^2(\mathbb{T}, d\mu, \mathfrak{k})$ is denoted by $L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta))$ where $\mathfrak{k}(\zeta) := P(\zeta)\mathfrak{k}$ in the following and is called a direct integral of Hilbert spaces $\{\mathfrak{k}(\zeta)\}_{\zeta \in \mathbb{T}}$, cf.[4]. We recall if an orthogonal projection on $L^2(\mathbb{T}, d\mu, \mathfrak{k})$ commutes with $\mathcal{Z}$, then there is a measurable family $\{P(\zeta)\}_{\zeta \in \mathbb{T}}$ of orthogonal projections such that P is given by (85).

For any unitary operator U there is a separable Hilbert space $\mathfrak{k}$ and a Borel measure μ on $\mathbb{T}$ such that U is unitarily equivalent to a part of $\mathcal{Z}$. That means, there is an isometry $\Psi : \mathfrak{H} \longrightarrow L^2(\mathbb{T}, d\mu, \mathfrak{k})$ such that

$$\Psi U = \mathcal{Z} \Psi.$$

The operator $P = \Psi \Psi^*$ is an orthogonal projection on $L^2(\mathbb{T}, d\mu, \mathfrak{k})$ commuting with $\mathcal{Z}$. Hence there is a family of measurable orthogonal projections $\{P(\zeta)\}_{\zeta \in \mathbb{T}}$ such that P is given by (85). Notice that Ψ is an isometry acting from $\mathfrak{H}$ onto $L^2(\mathbb{T}, d\mu, \mathfrak{k})$. The multiplication operator $M := \mathcal{Z} \upharpoonright L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta))$,

$$(Mf)(\zeta) = \zeta f(\zeta), \quad f \in L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta)),$$

is unitarily equivalent to U. The triplet $\Pi(U) = \{L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta)), M, \Psi\}$ is called a spectral representation of U.

The existence of a spectral representation can be proved as follows. Let $\mu(\cdot)$ be a scalar measure defined on $\mathfrak{B}(\mathbb{T})$ such that the spectral measure $E(\cdot)$ of U,

$$U = \int_{\mathbb{T}} \zeta dE(\zeta),$$

is absolutely continuous with respect to $\mu(\cdot)$. Such a measure μ always exists. Indeed, let $C = C^*$ be a Hilbert-Schmidt operator such that $\mathfrak{H} = \mathcal{H}_C(U) := \mathrm{clospan}\{E(\delta)\mathrm{ran}(C) : \delta \in \mathcal{B}(\mathbb{T})\}$ where $E(\cdot)$ is the spectral measure of U. We set

$$\mu(\delta) := \mathrm{tr}(CE(\delta)C), \quad \delta \in \mathfrak{B}(\mathbb{T}).$$

Obviously, the spectral measure $E(\cdot)$ is absolutely continuous with respect to $\mu(\cdot)$. In fact, both measures are equivalent.

Moreover, the operator-valued measure $\Sigma(\delta) := CE(\delta)C$, $\delta \in \mathfrak{B}(\mathbb{T})$, is absolutely continuous with respect to $\mu(\cdot)$ and takes values in $\mathfrak{L}_1(\mathfrak{H})$. Since $\mathfrak{L}_1(\mathfrak{H})$ has the Radon-Nikodym property $\Sigma(\cdot)$ admits a Radon-Nikodym derivative $\Upsilon(\cdot)$ of $\Sigma(\cdot)$ exists with respect to $\mu(\cdot)$, belongs to $\Upsilon(\zeta) \in \mathfrak{L}_1(\mathfrak{H})$ for a.e. $\zeta \in \mathbb{T}$ and satisfies $\Upsilon(\zeta) \geq 0$ for a.e. $\zeta \in \mathbb{T}$ with respect to μ. Hence we have

$$\Sigma(\delta) = \int_{\delta} \Upsilon(\zeta) d\mu(\zeta)$$

for any Borel set $\delta \in \mathfrak{B}(\mathbb{T})$. We set $\mathfrak{k}(\zeta) := \mathrm{ran}(\Upsilon(\zeta)) \subseteq \mathfrak{k}$, $\zeta \in \mathbb{T}$, which defines a measurable family of subspaces of $\mathfrak{k} := \mathrm{ran}(C)$. That means, the corresponding family of orthogonal projections from $\mathfrak{k}$ onto $\mathfrak{k}(\zeta)$ is measurable with respect to $\mu(\cdot)$.

Lemma A.1. *Let $L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta))$ and $\Upsilon(\zeta)$ be as above. Further, let Ψ be the linear extension of the mapping*

$$\big(\Psi E(\delta)Cf\big)(\zeta) = \chi_{\delta}(\zeta)\sqrt{\Upsilon(\zeta)}f, \quad \zeta \in \mathbb{T}, \quad f \in \mathfrak{H}.$$

If $\mathfrak{H} = \mathcal{H}_C(U)$, then $\Pi(U) = \{L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta)), M, \Psi\}$ is a spectral representation of U.

Proof. Obviously, we have

$$\|\Psi E(\delta)Cf\|^2_{L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k})} = \int_{\delta} \|\sqrt{\Upsilon(\zeta)}f\|^2_{\mathfrak{k}} d\mu(\zeta) = (\Sigma(\delta)f, f), \quad f \in \mathfrak{H}.$$

Hence Ψ is an isometry action from $\mathfrak{H}_C(U)$ into $L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k})$ with range $L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta))$. Since $\mathfrak{H} = \mathfrak{H}_C(U)$ one gets an isometry acting from $\mathfrak{H}$ onto $L^2(\mathbb{T}, d\mu(\zeta), \mathfrak{k}(\zeta))$. Moreover, by

$$(\Psi \int_{\mathbb{T}} U dE(\zeta)Cf)(\zeta) = \zeta\sqrt{\Upsilon(\zeta)}f, \quad \zeta \in \mathbb{T}, \quad f \in \mathfrak{H},$$

we get $\Psi U = \mathcal{Z}\Psi$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

The integer function $N_U : \mathbb{T} \longrightarrow \overline{\mathbb{N}}_0 := \{0, 1, 2, \ldots, \infty\}$, $N_U(\zeta) := \dim(\mathfrak{k}(\zeta))$, is called the spectral multiplicity function of U. We note that the family $\{\mathfrak{k}(\zeta)\}_{\zeta \in \mathbb{T}}$ and the spectral multiplicity function N_U are defined only a.e. with respect to μ. Furthermore, it can happen that $\mathfrak{k}(\zeta) = \{0\}$ for $\zeta \in \mathbb{T}$ which yields $N_U(\zeta) = 0$. We set $\mathrm{supp}\,(N_U) := \{\zeta \in \mathbb{T} : N_U(\zeta) > 0\}$ and introduce the measure $\mu_U := \chi_{\mathrm{supp}\,(N_U)}\mu$ which is absolutely continuous with respect to μ.

Let U and $\widetilde{U}$ be unitary operators and let $\Pi(U) = \{L^2(\mathbb{T}, d\mu, \mathfrak{k}(\zeta)), M, \Psi\}$ and $\widetilde{\Pi}(\widetilde{U}) = \{L^2(\mathbb{T}, d\widetilde{\mu}(\zeta), \widetilde{\mathfrak{k}}(\zeta)), \widetilde{M}, \widetilde{\Psi}\}$ be spectral representations, respectively. The operators $\widetilde{U}$ and U are unitary equivalent if and only if $\widetilde{\mu}_{\widetilde{U}}$ and μ_U are equivalent and $N_{\widetilde{U}}(\zeta) = N_U(\zeta)$ a.e. with respect to μ_U. The unitary operator U is called of constant spectral multiplicity $k \in \overline{\mathbb{N}} := \{1, 2, \ldots, \infty\}$ if $N_U(\zeta) = k$ a.e. with respect to μ_U.

B Spectral representation for U^{ac}

In the paper we mainly need a spectral representation of the absolutely continuous part U^{ac} of a unitary operator U. In this case we choose $\mu = \nu$ where ν is the Haar measure on $\mathbb{T}$. In this case the construction above simplifies as follows:

As above, let $C = C^* \in \mathfrak{L}_2(\mathfrak{H})$ be a Hilbert-Schmidt operator on $\mathfrak{H}$. Since $C \in \mathfrak{L}_2(\mathfrak{H})$ we define by $\Sigma^{ac} := CE_0^{\mathsf{ac}}(\cdot)C$ a $\mathfrak{L}_1$–valued measure on $\mathbb{T}$ which is absolutely continuous with respect to the Haar measure ν on $\mathbb{T}$. Its Radon-Nikodym derivative is denoted by $Y(\cdot)$.

Let us define a measurable family of subspaces by $\mathfrak{h}(\zeta)$ by setting $\mathfrak{h}(\zeta) := \mathrm{clo}\{\mathrm{ran}(Y(\zeta))\} \subseteq \mathfrak{h}$ in $\mathfrak{h} = \mathrm{clo}(\mathrm{ran}(C))$. With this family we associate the direct integral $L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$.

Lemma B.1. *Let $L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ and $Y(\zeta)$ as above. Further let Φ be the linear extension of the mapping*

$$\left(\Phi E^{\mathsf{ac}}(\zeta)Cf\right)(\zeta) = \chi_\delta(\zeta)\sqrt{Y(\zeta)}f, \quad \zeta \in \mathbb{T}, \quad f \in \mathfrak{H}.$$

If the condition $\mathfrak{H}^{ac}(U) = \mathcal{H}_C^{ac} := \mathrm{clospan}\{E^{ac}(\delta)\mathrm{ran}(C) : \delta \in \mathcal{B}(\mathbb{T})\}$ is satisfied, then $\Pi(U^{ac}) := \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$ defines a spectral representation of U^{ac}.

The proof is similar to that one of Lemma A.1. If the condition $\mathfrak{H}_C^{ac} = \mathcal{H}^{ac}(U)$ is not satisfied, then $\Pi(U^{ac}) = \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$ is not a spectral representation of U^{ac} but of $U_C^{ac} := U \upharpoonright \mathcal{H}_C^{ac}$. Notice that $\mathfrak{H}_C^{ac} \subseteq \mathfrak{H}^{ac}(U)$ reduces U^{ac}.

The following Lemma describes the action of the transformation Φ and is also valid for this extension of the spectral representation of Lemma B.1.

Lemma B.2. *Let $X : \mathbb{T} \to \mathfrak{B}(\mathfrak{H})$ be strongly continuous. If the operator spectral integral*

$$Lf = \int_{\mathbb{T}} \mathsf{d}E^{\mathsf{ac}}(\zeta)CX(\zeta)f, \qquad f \in \mathfrak{H},$$

exists, then

$$(\Phi Lf)(\zeta) = \sqrt{Y(\zeta)}X(\zeta)f, \qquad \zeta \in \mathbb{T}, \qquad f \in \mathfrak{H}, \tag{86}$$

holds. Furthermore,

$$L^* f := \int_{\mathbb{T}} X^*(\zeta)C\mathsf{d}E_0^{\mathsf{ac}}(\zeta)f$$

and

$$L^*\Phi^*\widehat{f} = \int_{\mathbb{T}} \mathsf{d}\lambda X^*(\zeta)\sqrt{Y(\zeta)}\widehat{f}(\zeta), \qquad f = \Phi^*\widehat{f} \in \mathfrak{H}^{\mathsf{ac}}. \tag{87}$$

Proof. Let $\mathcal{J}_\epsilon$, $\epsilon > 0$, be a family of partitions of $\mathbb{T}$ such that $\sup_{\Xi \in \mathcal{J}_\epsilon} |\Xi| = \epsilon$. Let further $\zeta_\epsilon : \mathcal{J}_\epsilon \to \mathbb{T}$ satisfy $\zeta_\epsilon(\Xi) \in \Xi$ for all $\Xi \in \mathcal{J}_\epsilon$. Then for

$$Lf := \int_{\mathbb{T}} \mathsf{d}E^{\mathsf{ac}}(\zeta)CX(\zeta)f, \qquad f \in \mathfrak{H},$$

we have

$$Lf = \lim_{\epsilon \to 0} \sum_{\Xi \in \mathcal{J}_\epsilon} E^{\mathsf{ac}}(\Xi)CX(\zeta_\epsilon(\Xi))f.$$

by definition. Since Φ_0 is continuous and $\mathrm{ran}(L) \subset \mathcal{H}(C)$, we have

$$(\Phi Lf)(\lambda) = \lim_{\epsilon \to 0} \sum_{\Xi \in \mathcal{J}_\epsilon} \left(\Phi E^{\mathsf{ac}}(\Xi)CX(\lambda_\epsilon(\Xi))f\right)(\lambda)$$

$$= \lim_{\epsilon \to 0} \sum_{\Xi \in \mathcal{J}_\epsilon} \chi_\Xi(\lambda)\sqrt{Y(\lambda)}X(\lambda_\epsilon(\Xi))f$$

for a.e. $\zeta \in \mathbb{T}$. Now let $\Xi_\epsilon(\lambda)$ be the unique element in $\mathcal{J}_\epsilon$ for which $\lambda \in \Xi_\epsilon(\lambda)$. Since X is continuous, we obtain

$$(\Phi L f)(\lambda) = \lim_{\epsilon \to 0} \sqrt{Y(\lambda)} X(\lambda_\epsilon(\Xi_\epsilon(\lambda))) f = \sqrt{Y(\lambda)} X(\lambda) f.$$

The adjoint relation (87) follows easily from

$$\left\langle g, \int_{\mathbb{T}} X(\zeta) C \mathsf{d} E^{\mathsf{ac}}(\zeta) f \right\rangle = \left\langle \int_{\mathbb{T}} \mathsf{d} E^{\mathsf{ac}}(\zeta) C X^*(\zeta) g, f \right\rangle$$

$$\int_{\mathbb{T}} \mathsf{d}\lambda \left\langle \sqrt{Y(\zeta)} X^*(\zeta) g, (\Phi f)(\zeta) \right\rangle = \left\langle g, \int_{\mathbb{T}} \mathsf{d}\zeta X(\zeta) \sqrt{Y(\zeta)} (\Phi f)(\zeta) \right\rangle$$

for all $g \in \mathfrak{H}$. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ $\square$

C Spectral representation for H^{ac}

Let H be a self-adjoint operator on the separable Hilbert space $\mathfrak{H}$. We introduce its Cayley transform

$$U := (i - H)(i + H)^{-1}.$$

Obviously, we have

$$E_U(\delta) = E_H(\delta'), \quad \delta \in \mathcal{B}(\mathbb{T}), \quad \delta' = \{\lambda \in \mathbb{R} : e^{2i \arctan(\lambda)} \in \delta\}.$$

Let $\Pi(U^{ac}) = \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$. Let us introduce the direct integral $L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda))$ where $d\lambda$ is the Lebesgue measure on $\mathbb{R}$, and $\mathfrak{h}'(\lambda) := \mathfrak{h}(e^{2i \arctan(\lambda)})$. A straightforward computation shows that the linear map $F : L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)) \longrightarrow L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda))$,

$$\widehat{f}'(\lambda) := (F\widehat{f})(\lambda) := \sqrt{\frac{2}{1 + \lambda^2}} \widehat{f}(e^{2i \arctan(\lambda)}), \quad \lambda \in \mathbb{R},$$

$\widehat{f} \in L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda))$, defines an isometry acting from $L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ onto $L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda))$. Let $\{Q(\zeta)\}_{\zeta \in \mathbb{T}}$ be a measurable operator-valued function which defines a multiplication operator M_Q in the direct integral $L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. Setting

$$Q'(\lambda) = Q(e^{2i \arctan(\lambda)}), \quad \lambda \in \mathbb{R},$$

one easily defines a multiplication operator in $M_{Q'}$ in $L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda))$. It turns out that $M_{Q'} = F M_Q F^{-1}$. In particular, one gets that

$$F M_{\chi_\delta} F^{-1} = M_{\chi'_\delta}, \quad \delta \in \mathcal{B}(\mathbb{T}), \quad \delta' = \{\lambda \in \mathbb{R} : e^{2i \arctan(\lambda)} \in \delta\}.$$

the last relation immediately shows that $\Pi(H^{ac}) := \{L^2(\mathbb{R}, d\lambda, \mathfrak{h}'(\lambda)), M, \Phi'\}$, $\Phi' := F\Phi$, defines a spectral representation of the absolutely continuous part H^{ac} of H.

D Scattering matrix for unitary operators

Let $\mathfrak{H}$ be a separable Hilbert space and let U and U_0 be unitary operators such that

$$V := U - U_0 \in \mathfrak{L}_1(\mathfrak{H}). \tag{88}$$

where $\mathfrak{L}_1(\cdot)$ denotes the set of trace class operators in $\mathfrak{H}$. In the following we call the pair $\mathcal{S} = \{U, U_0\}$ of unitary operators satisfying (88) a $\mathfrak{L}_1$-scattering system.

If $\mathcal{S} = \{U, U_0\}$ is a $\mathfrak{L}_1$ scattering system, then the wave operators

$$\Omega_\pm := \Omega_\pm(U, U_0) := \mathsf{s}\text{-}\lim_{n \to \pm\infty} U^n U_0^{-n} P^{ac}(U_0)$$

exist and are complete. Completeness means that $\mathrm{ran}(\Omega_\pm) = \mathfrak{H}^{ac}(U)$ where $\mathfrak{H}^{ac}(U)$. The scattering operator S of the scattering system $\mathcal{S}$ is defined by

$$S := S(U, U_0) := \Omega_+^* \Omega_-.$$

In fact, the scattering operator acts only on $\mathfrak{H}^{ac}(U_0)$ and is unitary there. Moreover, it commutes with U_0.

Let $\Pi(U_0^{ac}) = \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$ be a spectral representation of the absolutely continuous part U_0^{ac} of U_0, cf. Appendix B. Since the scattering operator S is unitary on $\mathfrak{H}^{ac}(U_0)$ and commutes with U_0^{ac} there is a measurable family $\{S(\zeta)\}_{\zeta \in \mathbb{T}}$ of unitary operator on $\mathfrak{h}(\zeta)$ such that S is unitary equivalent to M_S,

$$(M_S f)(\zeta) = S(\zeta) f(\zeta), \quad f \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)),$$

that is $S = \Phi^{-1} M_S \Phi$. The family $S(\zeta)$ of unitary operators is called the scattering matrix of the scattering system $\mathcal{S}$.

At first we prove a technical lemma.

Lemma D.1. *Let $\mathcal{S} = \{U, U_0\}$ be $\mathfrak{L}_1$-scattering system. Then there is a bounded self-adjoint Hilbert-Schmidt operator C and a bounded operator G such that the representation*

$$V := U - U_0 = CGC \tag{89}$$

is valid.

Proof. Let $V = V_R + iV_I$ where where $V_R := \frac{1}{2}(V + V^*)$ and $V_I := \frac{1}{2i}(V^* - V^*)$. Obviously, one has $V_R := V_R^* \in \mathfrak{L}_1(\mathfrak{H})$. and $V_I = V_I^* \in \mathfrak{L}_1(\mathfrak{H})$. Let $C_R := |V_R|^{1/2}$ and $C_I := |V_I|^{1/2}$. Then

$$V_R = C_R G_R C_R \quad \text{and} \quad V_I = C_I G_I C_I \tag{90}$$

where $G_R := \mathrm{sign}(V_R)$ and $G_I := \mathrm{sign}(V_I)$. We set

$$C := (|V_R| + |V_I|)^{1/2}.$$

Obviously, we have

$$\|C_R f\|^2 = (|V_R|f, f) \le ((|V_R| + |V_I|)f, f) = \|Cf\|^2, \quad f \in \mathfrak{H}.$$

Hence there is a contraction Γ_R such that $C_R = \Gamma_R C$ and $C_R = C\Gamma_R^*$. Similarly, there is a contraction Γ_I such that $C_I = \Gamma_I C_I$ and $C_I = C_I \Gamma_I^*$. From (90) we find

$$V = C(\Gamma_R^* G_R \Gamma_R + i\Gamma_I^* G_I \Gamma_I)C.$$

Setting $G := \Gamma_R^* G_R \Gamma_R + i\Gamma_I^* G_I \Gamma_I$ we prove (89). $\qquad\square$

We define the Abel pre-wave operators by

$$\begin{aligned}
\Omega_+(r) &:= (1-r)\sum_{n=0}^\infty r^n U^n U_0^{-n} P_0^{ac}, \\
\Omega_-(r) &:= (1-r)\sum_{n=0}^\infty r^n U^{-n} U_0^n P_0^{ac},
\end{aligned} \tag{91}$$

$r \in [0, 1)$, where we have used the abbreviation $P_0^{ac} := P^{ac}(U_0)$. It holds

$$\Omega_\pm = s\text{-}\lim_{r \uparrow 1} \Omega_\pm(r).$$

Let $E_0(\cdot)$ be spectral measure of U_0 defined on the Borel subsets of $\mathbb{T}$. We set $E_0^{ac}(\cdot) := P^{ac}(U_0)E_0(\cdot)$. A straightforward computation gives

$$\Omega_+(r) := P_0^{ac} + r \int_\mathbb{T} \frac{\overline{\zeta}}{I - r\overline{\zeta}U} V dE_0^{ac}(\zeta), \tag{92}$$

$$\Omega_-(r) := P_0^{ac} - r \int_\mathbb{T} \frac{U^*}{I - r\zeta U^*} V dE_0^{ac}(\zeta). \tag{93}$$

Using $U^*V = -V^*U_0$ we find

$$\Omega_-(r) := P_0^{ac} + r \int_{\mathbb{T}} \frac{\zeta}{I - r\zeta U^*} V^* dE_0^{ac}(\zeta). \tag{94}$$

Furthermore, from (92) and (94) we get

$$\Omega_+(r)^* = P_0^{ac} + r \int_{\mathbb{T}} dE_0^{ac}(\zeta) V^* \frac{\zeta}{I - r\zeta U^*} \tag{95}$$

$$\Omega_-(r)^* = P_0^{ac} + r \int_{\mathbb{T}} dE_0^{ac}(\zeta) V \frac{\overline{\zeta}}{I - r\overline{\zeta} U} \tag{96}$$

Notice that $w\text{-}\lim_{r\uparrow 1} \Omega_+(r)^* = \Omega_+^*$. Similarly, we find the representations

$$\Omega_+(r) = P_0^{ac} + r \int_{\mathbb{T}} dE(\zeta) V \frac{U_0^*}{I - r\zeta U_0^*} P_0^{ac}$$

$$\Omega_-(r) = P_0^{ac} - r \int_{\mathbb{T}} dE(\zeta) V \frac{\overline{\zeta}}{I - r\overline{\zeta} U_0} P_0^{ac}.$$

Using again $U^*V = -V^*U_0$ we get

$$\Omega_+(r) = P_0^{ac} - r \int_{\mathbb{T}} dE(\zeta) V^* \frac{\zeta}{(I - r\zeta U_0^*)} P_0^{ac} \tag{97}$$

$$\Omega_-(r) = P_0^{ac} + r \int_{\mathbb{T}} dE(\zeta) V^* \frac{U_0}{I - r\overline{\zeta} U_0} P_0^{ac}. \tag{98}$$

We consider the transition operator $T := \frac{1}{2i\pi}(P_0^{ac} - S)$. Notice that

$$S = P^{ac}(U_0) - 2\pi i T.$$

In fact the operator T acts only on $\mathfrak{H}^{ac}(U_0)$. Since the scattering operator S commutes with U_0 the transition operator T also commutes with U_0. With respect to the spectral representation $\Pi(U_0^{ac}) = \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$ the transition operator T takes the form of a multiplication operator M_T induced by a measurable family $\{T(\zeta)\}_{\zeta \in \mathbb{T}}$ of bounded operators. Obviously, we have

$$S(\lambda) = I_{\mathfrak{h}(\zeta)} - 2\pi i T(\zeta) \tag{99}$$

for a.e. $\zeta \in \mathbb{T}$. The family $T(\zeta)$ of bounded operators is called the transition matrix of the scattering system $\mathcal{S}$. We are going to compute the measurable family $\{T(\zeta)\}_{\zeta \in \mathbb{T}}$.

Theorem D.2. *Let $\mathcal{S} = \{U, U_0\}$ be a $\mathfrak{L}_1$-scattering system. With respect to the spectral representation $\Pi(U_0^{ac}) = \{L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)), M, \Phi\}$ of U_0^{ac}, cf. Appendix B, the family of transition matrices $\{T(\zeta)\}_{\zeta \in \mathbb{T}}$ admits the representation*

$$T(\zeta) = i\zeta \sqrt{Y(\zeta)} Z(\zeta) \sqrt{Y(\zeta)} \tag{100}$$

for a.e. $\zeta \in \mathbb{T}$ with respect to ν where $Z(\zeta) := \text{o-}\lim_{r\uparrow 1} Z(r\zeta)$ and

$$Z(\xi) := G^* + G^* C \frac{\xi}{I - \xi U^*} C G^*, \quad \xi \in \mathbb{D} := \{z \in \mathbb{C} : |\xi| < 1\}. \tag{101}$$

Proof. Obviously we have

$$T = \frac{1}{2i\pi} \Omega_+^* (\Omega_+ - \Omega_-).$$

We set

$$T(r) = \frac{1}{2i\pi} \Omega_+^* (\Omega_+(r) - \Omega_-(r)).$$

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Notice that $T = s\text{-}\lim_{r\uparrow 1} T(r)$. Using the representations (97) and (98) we get

$$T(r) = i\frac{r}{2\pi}\Omega_+^* \left\{ \int_{\mathbb{T}} dE(\xi) V^* \frac{\xi}{I - r\xi U_0^*} + \int_{\mathbb{T}} dE(\xi) V^* \frac{U_0}{I - r\bar{\xi}U_0} \right\} P_0^{ac}$$

which yields

$$T(r) = i\frac{r}{2\pi(1 + r)}(1 - r^2) \int_{\mathbb{T}} dE_0^{ac}(\xi)\Omega_+^* V^* \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac}.$$

Let us introduce the notation

$$T(r, s) := i\frac{r}{1 + r}\frac{1 - r^2}{2\pi} \int_{\mathbb{T}} dE_0^{ac}(\xi)\Omega_+^*(s) V^* \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac}, \quad 0 \le r, s < 1. \tag{102}$$

Since $w\text{-}\lim_{s\uparrow 1} \Omega_+^*(s) = \Omega_+^*$ it seems natural to expect that $w\text{-}\lim_{s\uparrow 1} T(r, s) = T(r)$ for $0 \le r < 1$. Indeed, integrating by parts we get

$$\int_{\mathbb{T}} dE_0^{ac}(\xi)\Omega_+^* V^* \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac} =$$

$$\Omega_+^* V^* \frac{U_0 - 1}{|I + rU_0^*|^2} P_0^{ac} - \int_{\mathbb{T}} E_0^{ac}(\xi)\Omega_+^* V^* \frac{\partial}{\partial \xi} \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac} d\nu(\xi)$$

and

$$\int_{\mathbb{T}} dE_0^{ac}(\xi)\Omega_+^*(s) V^* \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac} =$$

$$\Omega_+^*(s) V^* \frac{U_0 - 1}{|I + rU_0^*|^2} P_0^{ac} - \int_{\mathbb{T}} E_0^{ac}(\xi)\Omega_+^*(s) V^* \frac{\partial}{\partial \xi} \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac} d\nu(\xi).$$

Because $\frac{\partial}{\partial \xi} \frac{U_0 + \xi}{|I - r\xi U_0^*|^2}$ is bounded for $r \in [0, 1)$ we find that

$$w\text{-}\lim_{s\uparrow 1} \int_{\mathbb{T}} dE_0^{ac}(\xi)\Omega_+^*(s) V^* \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac} =$$

$$\Omega_+^* V^* \frac{U_0 - 1}{|I + rU_0^*|^2} P_0^{ac} - \int_{\mathbb{T}} E_0^{ac}(\xi)\Omega_+^* V^* \frac{\partial}{\partial \xi} \frac{U_0 + \xi}{|I - r\xi U_0^*|^2} P_0^{ac} d\nu(\xi)$$

which proves $w\text{-}\lim_{s\uparrow 1} T(r, s) = T(r)$ for $0 \le r < 1$. From (95) we get

$$\Omega_+(s)^* = \int_{\mathbb{T}} dE_0^{ac}(\zeta) \left\{ I + s V^* \frac{\zeta}{I - s\zeta U^*} \right\}. \tag{103}$$

Inserting (103) into (102) we obtain

$$T(r, s) = i\frac{r}{1 + r}\frac{1 - r^2}{2\pi} \int_{\mathbb{T}} dE_0^{ac}(\zeta) \left\{ I + s V^* \frac{\zeta}{I - s\zeta U^*} \right\} V^* \frac{U_0 + \zeta}{|I - r\zeta U_0^*|^2} P_0^{ac}$$

where $\zeta \in \mathbb{T}$. Using (89) and the notation (101) we get

$$T(r, s) = i\frac{r}{1 + r}\frac{1 - r^2}{2\pi} \int_{\mathbb{T}} dE_0^{ac}(\zeta) CZ(s\zeta) C \frac{U_0 + \zeta}{|I - r\zeta U_0^*|^2} P_0^{ac}. \tag{104}$$

Inserting the representation

$$\frac{U_0 + \zeta}{|I - r\zeta U_0^*|^2} P_0^{ac} = \int_{\mathbb{T}} \frac{\xi + \zeta}{|1 - r\zeta\bar{\xi}|^2} dE_0^{ac}(\xi)$$

into (104) we find

$$T(r, s) = i\frac{r}{1 + r} \int_{\mathbb{T}} dE_0^{ac}(\zeta) CZ(s\zeta)\frac{1 - r^2}{2\pi} \int_{\mathbb{T}} \frac{\xi + \zeta}{|1 - r\zeta\bar{\xi}|^2} C dE_0^{ac}(\xi)$$

which leads to

$$T(r,s) = i\frac{r}{1+r}\int_{\mathbb{T}} dE_0^{ac}(\zeta) CZ(s\zeta)\zeta \ \frac{1-r^2}{2\pi}\int_{\mathbb{T}}\frac{\xi\overline{\zeta}+1}{|1-r\zeta\overline{\xi}|^2}CdE_0^{ac}(\xi).$$

Applying the map $\Phi : \mathfrak{H}^{ac}(U_0) \longrightarrow L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ we obtain

$$(\Phi T(r,s)\Phi^{-1}\,\widehat{f})(\zeta) =$$
$$i\frac{r}{1+r}\sqrt{Y(\zeta)}Z(s\zeta)\zeta \ \frac{1-r^2}{2\pi}\int_{\mathbb{T}}\frac{\xi\overline{\zeta}+1}{|1-r\zeta\overline{\xi}|^2}\sqrt{Y(\xi)}\,\widehat{f}(\xi)d\nu(\xi)$$

where $\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. We set

$$X(s;\zeta) := \sqrt{Y(\zeta)}Z(s\zeta), \quad \zeta \in \mathbb{T}, \quad 0 \le s < 1. \tag{105}$$

Notice that $X(s;\zeta) \in \mathfrak{L}_2(\mathfrak{H})$ for a.e. $\zeta \in \mathbb{T}$. Since $X(s) := \mathfrak{L}_2 - \lim_{s\uparrow 1} X(s;\zeta) = \sqrt{Y(s)}Z(s)$ exists for a.e. $\zeta \in \mathbb{T}$ there is a Borel subset $\Delta(\varepsilon) \subseteq \mathbb{T}$ for every $\varepsilon > 0$ such that $\nu(\Delta(\varepsilon)) < \varepsilon$ and

$$C_X(\varepsilon) := \sup\{\|X(s;\zeta)\|_{\mathfrak{L}_2} : \zeta \in \mathbb{T} \setminus \Delta(\varepsilon), \quad 0 \le s < 1\} < \infty \tag{106}$$

is valid. We note the existence of the set $\Delta(\varepsilon)$ follows from Egorov's theorem.

Using that observation we get

$$(\Phi E_0^{ac}(\mathbb{T} \setminus \Delta(\varepsilon))T(r)\Phi^{-1}\,\widehat{f})(\zeta) = w\text{-}\lim_{s\uparrow 1}(\Phi E_0^{ac}(\mathbb{T} \setminus \Delta)(\varepsilon))T(r,s)\Phi^{-1}\,\widehat{f})(\zeta)$$

$$= i\zeta\frac{r}{1+r}\chi_{\mathbb{T}\setminus\Delta(\varepsilon)}(\zeta)\sqrt{Y(\zeta)}Z(\zeta)\ \frac{1-r^2}{2\pi}\int_{\mathbb{T}}\frac{\xi\overline{\zeta}+1}{|1-r\zeta\overline{\xi}|^2}\sqrt{Y(\xi)}\,\widehat{f}(\xi)d\nu(\xi)$$

for a.e. $\zeta \in \mathbb{T}$ with respect to ν and $\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. Finally, taking the limit $r \uparrow 1$ we get

$$(\Phi E_0^{ac}(\mathbb{T} \setminus \Delta(\varepsilon))T\Phi^{-1}\,\widehat{f})(\zeta) =$$
$$\lim_{r\uparrow 1}\Phi E_0^{ac}(\mathbb{T} \setminus \Delta(\varepsilon))T(r)\Phi^{-1}\,\widehat{f})(\zeta) = i\zeta\chi_{\mathbb{T}\setminus\Delta(\varepsilon)}(\zeta)\sqrt{Y(\zeta)}Z(\zeta)\ \sqrt{Y(\zeta)}\,\widehat{f}(\zeta)$$

for a.e. $\zeta \in \mathbb{T}$ with respect to ν and $\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ where it was used that

$$\widehat{g}(\zeta) = \frac{1}{2}\lim_{r\uparrow 1}\frac{1-r^2}{2\pi}\int_{\mathbb{T}}\frac{\xi\overline{\zeta}+1}{|1-r\zeta\overline{\xi}|^2}\,\widehat{g}(\xi)d\nu(\xi), \quad \widehat{g} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta)),$$

in the L^2-sense, see [16, Section I.D.2]. If $\widehat{f}(\zeta) \in L^\infty(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$, then $\sqrt{Y(\zeta)}\,\widehat{f}(\zeta) \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$. Hence we find that

$$(T(\zeta)\,\widehat{f})(\zeta) = i\zeta\sqrt{Y(\zeta)}Z(\zeta)\ \sqrt{Y(\zeta)}\,\widehat{f}(\zeta),$$

for a.e. $\zeta \in \mathbb{T} \setminus \Delta(\varepsilon)$ and $f \in L^\infty(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ which yields (100) for a.e. $\zeta \in \mathbb{T} \setminus \Delta(\varepsilon)$. Since ε can be chosen arbitrary small we we prove (100). □

From (99) and (100) we get that the scattering matrix admits the representation

$$S(\zeta) = I_{\mathfrak{h}(\zeta)} + 2\pi\zeta\sqrt{Y(\zeta)}Z(\zeta)\sqrt{Y(\zeta)}$$

for a.e. $\zeta \in \mathbb{T}$. Since $\|S(\zeta)\|_{\mathfrak{h}(\zeta)} = 1$ for a.e. $\zeta \in \mathbb{T}$ we get $\|S(\zeta) - I_{\mathfrak{h}(\zeta)}\|_{\mathfrak{h}(\zeta)} \le 2$ for a.e $\zeta \in \mathbb{T}$ which yields

$$\|\sqrt{Y(\zeta)}Z(\zeta)\sqrt{Y(\zeta)}\|_{\mathfrak{h}(\zeta)} \le \frac{1}{\pi}$$

for a.e. $\zeta \in \mathbb{T}$. In fact, this estimate can be proved directly.

Corollary D.3. *Let the assumptions of Theorem D.2 be satisfied. Then the following holds:*

(i) *For $\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ we have*

$$(\Phi\Omega_-^*(r)VP^{ac}(U_0)\Phi^{-1}\widehat{f})(\zeta) = \int_{\mathbb{T}} K(r;\zeta,\xi)\,\widehat{f}(\xi)d\nu(\xi), \quad r \in [0,1), \tag{107}$$

for a.e. $\zeta \in \mathbb{T}$ with respect to ν where $K(r;\zeta,\xi) := \sqrt{Y(\zeta)}Z(r\zeta)^*\sqrt{Y(\xi)}, \zeta, \xi \in \mathbb{T}$.

(ii) *For $\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ we have*

$$(\Phi\Omega_-^*VP^{ac}(U_0)\Phi^{-1}\widehat{f})(\zeta) = \int_{\mathbb{T}} K(\zeta,\xi)\,\widehat{f}(\xi)d\nu(\xi). \tag{108}$$

for a.e. $\zeta \in \mathbb{T}$ with respect to ν where $K(\zeta,\xi) := \sqrt{Y(\zeta)}\,Z(\zeta)^*\sqrt{Y(\xi)}, \zeta, \xi \in \mathbb{T}$.

(iii) *For a.e. $\zeta \in \mathbb{T}$ with respect to ν one has the representation $T(\zeta) = i\zeta\,K(\zeta,\zeta)^*$. Moreover, $T(\zeta) \in \mathfrak{L}_1(\mathfrak{h}(\lambda))$ for a.e $\zeta \in \mathbb{T}$ with respect to ν, $\|T(\zeta)\|_{\mathfrak{S}_1} \in L^1(\mathbb{T}, d\nu(\zeta))$ and*

$$\int_{\mathbb{T}} \|T(\zeta)\|_{\mathfrak{L}_1}d\nu(\zeta) \leq \|V\|_{\mathfrak{L}_1}. \tag{109}$$

In addition one has

$$\mathrm{tr}(\Omega_-^*V) = \int_{\mathbb{T}} \mathrm{tr}(K(\zeta,\zeta))d\nu(\zeta) = i\int_{\mathbb{T}} \zeta\,\mathrm{tr}(T(\zeta)^*)d\nu(\zeta). \tag{110}$$

Proof. (i) Let $K(r) := \Omega_-^*(r)V$. Using (96) we get

$$K(r)P_0^{ac} = \left\{ P_0^{ac} + r\int_{\mathbb{T}} dE_0^{ac}(\zeta)V\frac{\overline{\zeta}}{I - r\overline{\zeta}U} \right\}VP_0^{ac}$$

which leads to

$$K(r)P_0^{ac} = \int_{\mathbb{T}} dE_0^{ac}(\zeta)C\left\{ G + rGC\frac{\overline{\zeta}}{I - r\overline{\zeta}U}CG \right\}\int_{\mathbb{T}} CdE_0^{ac}(\xi).$$

From (101) we get

$$Z(r\zeta)^* = G + rGC\frac{\overline{\zeta}}{I - r\overline{\zeta}U}CG$$

which yields

$$K(r)P_0^{ac} = \int_{\mathbb{T}} dE_0^{ac}(\zeta)CZ(r\zeta)^*\int_{\mathbb{T}} CdE_0^{ac}(\xi).$$

Thus

$$(\Phi K(r)P_0^{ac}\Phi^{-1}\widehat{f})(\zeta) = \sqrt{Y(\zeta)}Z(r\zeta)^*\int_{\mathbb{T}} \sqrt{Y(\xi)}\,\widehat{f}(\xi)d\nu(\xi),$$

$\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$ which verifies (107).

(ii) Following the proof of Theorem D.2 we set

$$X_*(r;\zeta) := \sqrt{Y(\zeta)}Z(r\zeta)^*, \quad \zeta \in \mathbb{T}, \quad 0 \leq r < 1. \tag{111}$$

As above, using the existence of $X_*(\zeta) := \mathfrak{L}_2 - \lim_{r\uparrow 1} X(r;\zeta) = \sqrt{Y(\zeta)}Z(\zeta)^*$ for a.e. $\zeta \in \mathbb{T}$ with respect to ν we find that for each $\varepsilon > 0$ there is a Borel subset $\Delta_*(\varepsilon) \subseteq \mathbb{T}$ satisfying $\nu(\Delta_*(\varepsilon)) < \varepsilon$ such that the condition

$$C_{X_*}(\varepsilon) := \sup\left\{ \|X_*(s;\zeta)\|_{\mathfrak{L}_2} : \zeta \in \mathbb{T} \setminus \Delta_*(\varepsilon), \quad 0 \leq s < 1 \right\} < \infty. \tag{112}$$

Using $K := w\text{-}\lim_{r\uparrow 1} K(r) = \Omega_-^* V$ we get

$$(\Phi E^{ac}(\mathbb{T} \setminus \Delta_*(\varepsilon))\Omega_-^* V P_0^{ac} \Phi^{-1} \widehat{f})(\zeta) =$$

$$w\text{-}\lim_{r\uparrow 1}(\Phi E^{ac}(\mathbb{T} \setminus \Delta_*(\varepsilon))\Omega_-^*(r) V P_0^{ac} \Phi^{-1} \widehat{f})(\zeta) =$$

$$\chi_{\mathbb{T}\setminus\Delta_*(\varepsilon)}(\zeta)\sqrt{Y(\zeta)}Z(\zeta)^* \int_{\mathbb{T}} \sqrt{Y(\xi)}\, \widehat{f}(\xi)d\nu(\xi),$$

$\widehat{f} \in L^2(\mathbb{T}, d\nu(\zeta), \mathfrak{h}(\zeta))$, which proves (108) for a.e. $\zeta \in \mathbb{T} \setminus \Delta_*(\varepsilon)$ with respect to ν. Since ε is arbitrary (108) holds for a.e. $\zeta \in \mathbb{T}$.

(iii) By [24, Proposition 7.5.2] we find that $\|K(\zeta,\zeta)\|_{\mathfrak{L}_1} \in L^1(\mathbb{T}, d\nu(\zeta))$ and

$$\int_{\mathbb{T}} \|K(\zeta,\zeta)\|_{\mathfrak{L}_1} d\nu(\zeta) \leq \|K\|_{\mathfrak{L}_1}.$$

From (100) we get that $T(\zeta) = i\zeta K(\zeta,\zeta)$ for a.e. $\zeta \in \mathbb{T}$ with respect to ν. Thus $\|T(\zeta)\|_{\mathfrak{H}_1} \in L^1(\mathbb{T}, d\nu(\zeta))$ and (109) is valid. Using again [24, Proposition 7.5.2] we find

$$\text{tr}(\Omega_-^* V) = \text{tr}(K) = \int_{\mathbb{T}} \text{tr}(K(\zeta,\zeta))d\nu(\zeta).$$

By $T(\zeta) = i\zeta K(\zeta,\zeta)$ we prove (110). $\qquad\square$

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