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The Cayley transform applied to non-interacting quantum transport

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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.

Keywords: Landauer–Büttiker formula; Dissipative Schrödinger operators; Self-adjoint dilations; Dirac operators

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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

$$\operatorname{tr}\bigl(\Phi(H_0 + V) - \Phi(H_0)\bigr) = \int_{\mathbb{R}} \xi(\lambda)\Phi'(\lambda)\,d\lambda \tag{1.1}$$

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 (1.1) 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 Kreĭn, cf. [17]. In a first step Kreĭn 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

$$\operatorname{tr}\bigl(\Phi(H) - \Phi(H_0)\bigr) = \int_{\mathbb{R}} \xi(\lambda)\Phi'(\lambda)\,d\lambda \tag{1.2}$$

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

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

holds. In contrast to the spectral shift function defined by (1.2), the function $\xi(\cdot)$ defined by the last equation is now not unique and is only determined up to a real constant. To verify (1.2) Kreĭn firstly proved a trace formula (1.1) 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, Kreĭn was able to establish (1.2).

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

$$W_\pm(H, H_0) = s\text{-}\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}P^{ac}(H_0) \tag{1.3}$$

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–Kreĭn formula

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

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