Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

The effect of time-dependent coupling on non-equilibrium steady states

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

submitted: November 07, 2007

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

[2] Weierstraß-Institut für
Angewandte Analysis and Stochastik
Mohrenstr. 39
D-10117 Berlin, Germany
E-mail: neidhard@wias-berlin.de

[3] Université de la Méditerranée (Aix-Marseille II)
Centre de Physique Théorique - UMR 6207
Luminy - Case 907
F-13288 Marseille Cedex 9, France
E-mail: zagrebnov@cpt.univ-mrs.fr

No. 1267
Berlin 2007

2000 *Mathematics Subject Classification.* 46N55, 47N55, 47A40, 35L90, 47E05 .

Key words and phrases. non-equilibrium steady states, Landauer-Büttiker formula, Landau-Lifschitz formula, quantum Liouville equation, wave and scattering operator .

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

Consider (for simplicity) two one-dimensional semi-infinite leads coupled to a quantum well via time dependent point interactions. In the remote past the system is decoupled, and each of its components is at thermal equilibrium. In the remote future the system is fully coupled. We define and compute the non equilibrium steady state (NESS) generated by this evolution. We show that when restricted to the subspace of absolute continuity of the fully coupled system, the state does not depend at all on the switching. Moreover, we show that the stationary charge current has the same invariant property, and derive the Landau-Lifschitz and Landauer-Büttiker formulas.

Contents

1 Introduction

The goal of this paper is to construct and study non equilibrium steady states for systems containing quantum wells, and to describe the quantum transport of electrons through them. Even though our results can be generalized to higher dimensions, we choose for the moment to work in a (quasi) one dimensional setting; let us describe it in some more detail.

A quantum well consists of potential barriers which are supposed to confine particles. On both sides of the barriers are reservoirs of electrons. Carriers can pass through the barriers by tunneling. We are interested in the carrier transport through the barriers, as well as in the carrier distribution between these barriers. Models of such type are very often used to describe processes going on in nanoelectronic devices: quantum well lasers, resonant tunneling diodes, and nanotransistors, see [32].

The quasi one dimensional geometry assumes that the carriers can freely move in the plane orthogonal to the transport axis, but these degrees of freedom are integrated out. Thus we are dealing with an essentially one-dimensional physical system. To describe such a system we consider the transport model of a single band in a given spatially varying potential v, under the assumption that v and all other possible parameters of the model are constant outside a fixed interval (a, b), see [15, 16, 20].

More precisely, in the Hilbert space $\mathfrak{H} := L^2(\mathbb{R})$ we consider the Schrödinger operator

$$(Hf)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx}f(x) + V(x)f(x), \quad x \in \mathbb{R}, \tag{1.1}$$

with domain

$$\mathrm{Dom}\,(H) := \{f \in W^{1,2}(\mathbb{R}) : \frac{1}{M}f' \in W^{1,2}(\mathbb{R})\}. \tag{1.2}$$

It is assumed that the effective mass $M(x)$ and the real potential $V(x)$ admit decompositions of the form

$$M(x) := \begin{cases} m_a & x \in (-\infty, a] \\ m(x) & x \in (a, b) \\ m_b & x \in [b, \infty) \end{cases}, \tag{1.3}$$

$0 < m_a, m_b < \infty$, $m(x) > 0$, $x \in (a, b)$, $m + \frac{1}{m} \in L^\infty((a, b))$, and

$$V(x) := \begin{cases} v_a & x \in (-\infty, a] \\ v(x) & x \in (a, b) \\ v_b & x \in [b, \infty) \end{cases}, \quad v_a \geq v_b, \tag{1.4}$$

$v_a, v_b \in \mathbb{R}$, $v \in L^\infty((a, b))$. The quantum well is identified with the interval (a, b), (or physically, with the three-dimensional region $(a, b) \times \mathbb{R}^2$). The regions $(-\infty, a)$ and (b, ∞) (or physically $(-\infty, a) \times \mathbb{R}^2$ and $(b, \infty) \times \mathbb{R}^2$), are the reservoirs.

Schrödinger operators with step-like potentials were firstly considered by Buslaev and Fomin in [8]. For that reason we call them Buslaev-Fomin operators.

The inverse scattering problem for such Buslaev-Fomin operators was subsequently investigated in [1, 2, 3, 10, 11, 18].

In order to rigorously describe quantum transport in mesoscopic systems, these operators were firstly used by Pötz, see [28]. In [6], the Buslaev-Fomin operator was an important ingredient for a self-consistent quantum transmitting Schrödinger-Poisson system, which was used to describe quantum transport in tunneling diodes. In a further step, this was extended to a so-called hybrid model which consists of a classical drift-diffusion part and a quantum transmitting Schrödinger-Poisson part, see [7]. Hybrid models are effective tools of describing and calculating nanostructures like tunneling diodes, see [5].

To obtain a self-consistent description of carrier transport through quantum wells, one needs to know the carrier distribution between the barriers in order to put it into the Poisson equation for determining the electric field. Semiconductor devices are often modeled in this manner, see [17, 22, 29]. Important for that is a relation which assigns to each real potential $v \in L^\infty((a,b))$ a carrier density $u \in L^1((a,b))$. The (nonlinear) operator doing this is called the carrier density operator and is denoted by

$$\mathcal{N}(\cdot) : L^\infty((a,b)) \longrightarrow L^1((a,b)), \qquad \mathcal{N}(v) = u.$$

The problem of defining carrier density operators is reduced to the problem of finding appropriate density operators ϱ.

Definition 1.1 *A bounded non-negative operator ϱ in $L^2(\mathbb{R})$ is called a density operator or a state if the product $\varrho M(\chi_{(a,b)})$ is a trace class operator, where $M(\chi_{(a,b)})$ is the multiplication operator induced in $L^2(\mathbb{R})$ by the characteristic function $\chi_{(a,b)}$ of the interval (a,b).*

We note that in general a non-negative bounded operator is called a state if the operator itself is a trace class operator and is normalized to one, that is, $\mathrm{Tr}(\varrho) = 1$. In our case these conditions are relaxed to the condition that the product $\varrho M(\chi_{(a,b)})$ has to be trace class.

This weakening is necessary since we are interested in so-called steady density operators or steady states for Hamiltonians with continuous spectrum.

Definition 1.2 *A state ϱ is called a* steady state *for H if ϱ commutes with H, i.e., ϱ belongs to the commutant of the W^*-algebra generated by the spectral measure $E_H(\cdot)$ of H. A steady state is an* equilibrium state *if it belongs to the bicommutant of this algebra.*

Thus if H admits continuous spectrum, then a steady state cannot be of trace class unless it equals zero on the subspace of absolute continuity.

To give a description of all possible steady states, one has to introduce the spectral representation of H. Taking into account results of [6], it turns out that the operator H is unitarily equivalent to the multiplication M induced by the independent variable λ in the direct integral $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$,

$$\mathfrak{h}(\lambda) := \begin{cases} \mathbb{C}, & \lambda \in (-\infty, v_a] \\ \mathbb{C}^2, & \lambda \in (v_a, \infty) \end{cases}, \tag{1.5}$$

and (with the usual abuse of notation)

$$d\nu(\lambda) = \sum_{j=1}^{N} \delta(\lambda - \lambda_j) d\lambda + \chi_{[v_b,\infty)}(\lambda) d\lambda, \quad \lambda \in \mathbb{R},$$

where it is assumed $v_a \geq v_b$, and $\{\lambda_j\}_{j=1}^N$ denote the finite number of simple eigenvalues of H which are all situated below the threshold v_b. We note that

$$L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu) \simeq \oplus_{j=1}^N \mathbb{C} \oplus L^2([v_b, v_a], \mathbb{C}) \oplus L^2((v_a, \infty), \mathbb{C}^2).$$

The unitary operator $\Phi : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$ establishing the unitary equivalence of H and M is called the generalized Fourier transform.

If ϱ is a steady state for H, then there exists a ν-measurable function

$$\mathbb{R} \ni \lambda \mapsto \tilde{\rho}(\lambda) \in B(\mathfrak{h}(\lambda))$$

of non-negative bounded operators in $\mathfrak{h}(\lambda)$ such that $\nu - \sup_{\lambda \in \mathbb{R}} \|\tilde{\rho}(\lambda)\|_{\mathfrak{B}(\mathfrak{h}(\lambda))} < \infty$ and ϱ is unitarily equivalent to the multiplication operator $M(\tilde{\rho})$ induced by $\tilde{\rho}$ via the generalized Fourier transform

$$\varrho = \Phi^{-1} M(\tilde{\rho}) \Phi. \tag{1.6}$$

The measurable family $\{\tilde{\rho}(\lambda)\}_{\lambda \in \mathbb{R}}$ is uniquely determined by the steady state ϱ up to a ν-zero set and is called the distribution function of the steady state. In other words, there is an one-to-one correspondence between the set of steady states and the set of distribution functions. When ρ is an equilibrium state, then $\tilde{\rho}(\lambda)$ must be proportional with the identity operator in $\mathfrak{h}(\lambda)$, hence ρ must be a function of H. Let us note that the same distribution function can produce quite different steady states in $L^2(\mathbb{R})$. This is due to the fact that the generalized Fourier transform strongly dependents on H, in particular, on the potential v.

Having a steady state ϱ for H one defines the carrier density in accordance with [6] as the Radon-Nikodym derivative of the Lebesgue continuous measure $\mathbb{E}(\omega)$

$$\mathbb{E}(\omega) := \mathrm{Tr}(\varrho M(\chi_\omega))$$

where ω is a Borel subset of (a, b). The quantity $\mathbb{E}(\omega)$ can be regarded as the expectation value that the carriers are contained in ω. Therefore the carrier density u is defined by

$$u_\rho(x) := \frac{\mathbb{E}(dx)}{dx} = \frac{\mathrm{Tr}(\varrho M(\chi_{dx}))}{dx}, \quad x \in (a, b).$$

The carrier density operator $\mathcal{N}_\rho(\cdot) : L^\infty((a,b)) \longrightarrow L^1((a,b))$ is now defined as

$$\mathcal{N}_\rho(v) := u_\rho(x) \tag{1.7}$$

where $v \in L^\infty((a,b))$ is the potential of the operator H. The steady state ϱ is given by (1.6).

Therefore the self-consistent description of the carrier transport through quantum wells is obtained if there is a way to determine physically relevant distribution functions $\tilde{\rho}$. One goal of this paper is to propose a time-dependent procedure allowing to determine those functions.

1.1 The strategy

Let us describe the strategy. We start with a completely decoupled system which consists of three subsystems living in the Hilbert spaces

$$\mathfrak{H}_a := L^2((-\infty, a]), \quad \mathfrak{H}_\mathcal{I} := L^2(\mathcal{I}), \quad \mathfrak{H}_b := L^2([b, \infty)) \tag{1.8}$$

where $\mathcal{I} = (a,b)$. We note that

$$\mathfrak{H} = \mathfrak{H}_a \oplus \mathfrak{H}_\mathcal{I} \oplus \mathfrak{H}_b. \tag{1.9}$$

With $\mathfrak{H}_a$ we associate the Hamiltonian H_a

$$\begin{aligned} (H_a f)(x) &:= -\frac{1}{2m_a}\frac{d^2}{dx^2}f(x) + v_a f(x), & (1.10)\\ f \in \mathrm{Dom}\,(H_a) &:= \{f \in W^{2,2}((-\infty, a)) : f(a) = 0\} & (1.11) \end{aligned}$$

with $\mathfrak{H}_\mathcal{I}$ the Hamiltonian $H_\mathcal{I}$,

$$\begin{aligned} (H_\mathcal{I} f)(x) &:= -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x) + v(x)f(x), & (1.12)\\ f \in \mathrm{Dom}\,(H_\mathcal{I}) &:= \left\{ f \in W^{1,2}(\mathcal{I}) : \begin{array}{l} \frac{1}{m}f' \in W^{1,2}(\mathcal{I}) \\ f(a) = f(b) = 0 \end{array} \right\} & (1.13) \end{aligned}$$

and with $\mathfrak{H}_b$ the Hamiltonian H_b,

$$\begin{aligned} (H_b f)(x) &:= -\frac{1}{2m_b}\frac{d^2}{dx^2}f(x) + v_b f(x), & (1.14)\\ f \in \mathrm{Dom}\,(H_b) &:= \{f \in W^{2,2}((b, \infty) : f(b) = 0\}. & (1.15) \end{aligned}$$

In $\mathfrak{H}$ we set

$$H_D := H_a \oplus H_\mathcal{I} \oplus H_b \tag{1.16}$$

where the sub-index "D" indicates Dirichlet boundary conditions. The quantum subsystems $\{\mathfrak{H}_a, H_a\}$ and $\{\mathfrak{H}_b, H_b\}$ are called left- and right-hand reservoirs. The middle system $\{\mathfrak{H}_\mathcal{I}, H_\mathcal{I}\}$ is identified with a closed quantum well. We assume that

all three subsystems are at thermal equilibrium; according to Definition 1.2, the corresponding sub-states must be functions of their corresponding sub-Hamiltonians. The total state is the direct sum of the three sub-states.

One example borrowed from the physical literature, which takes into account the quasi one dimensional features of our problem is as follows. Assume the same temperature T. The equilibrium sub-states are ϱ_a, $\varrho_{\mathcal{I}}$ and ϱ_b where:

$$\varrho_a := \mathfrak{f}_a(H_a - \mu_a), \quad \varrho_{\mathcal{I}} := \mathfrak{f}_{\mathcal{I}}(H_{\mathcal{I}} - \mu_{\mathcal{I}}), \quad \varrho_b := \mathfrak{f}_b(H_b - \mu_b) \tag{1.17}$$

where

$$\mathfrak{f}_a(\lambda) := c_a \ln(1 + e^{-\beta\lambda}),\ \mathfrak{f}_{\mathcal{I}}(\lambda) := c_{\mathcal{I}} \ln(1 + e^{-\beta\lambda}),\ \mathfrak{f}_b(\lambda) := c_b \ln(1 + e^{-\beta\lambda}),$$

$\lambda \in \mathbb{R}$, $\beta := 1/(kT)$, k is the Boltzmann constant, μ_a and μ_b are the chemical potentials of left- and right-hand reservoirs and $\mu_{\mathcal{I}}$ the chemical potential of the quantum well. The constants c_a, $c_{\mathcal{I}}$ and c_b are given by

$$c_a := \frac{q\, m_a^*}{\pi\, \beta}, \quad c_{\mathcal{I}} := \frac{q\, m_{\mathcal{I}}^*}{\pi\, \beta}, \quad c_b := \frac{q\, m_b^*}{\pi\, \beta} \tag{1.18}$$

where m_a^*, $m_{\mathcal{I}}^*$ and m_b^* are the electronic effective masses appearing after integrating out the orthogonal degrees of freedom (see for more details [15, 16]).

We set

$$\varrho_D := \varrho_a \oplus \varrho_{\mathcal{I}} \oplus \varrho_b. \tag{1.19}$$

For the whole system $\{\mathfrak{H}, H_D\}$ the state ϱ_D is a steady state because ϱ_D commutes with H_D (see Definition 1.2). In general, the state ϱ_D cannot be represented as a function of H_D which is characteristic for equilibrium states, but it is the direct sum of equilibrium sub-states. In any case, ϱ_D is a special non-equilibrium steady state (NESS) for the system $\{\mathfrak{H}, H_D\}$. Now here comes the main question: can we construct a NESS for $\{\mathfrak{H}, H\}$ starting from ϱ_D?

Let us assume that at $t = -\infty$ the quantum system $\{\mathfrak{H}, H_D\}$ is described by the NESS ϱ_D. Then we connect in a time dependent manner the left- and right-hand reservoirs to the closed quantum well $\{\mathfrak{H}_{\mathcal{I}}, H_{\mathcal{I}}\}$. We assume that the connection process is described by the time-dependent Hamiltonian

$$H_\alpha(t) := H + e^{-\alpha t}\delta(x - a) + e^{-\alpha t}\delta(x - b), \quad t \in \mathbb{R}, \quad \alpha > 0. \tag{1.20}$$

The operator $H_\alpha(t)$ is defined by

$$(H_\alpha(t))f)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx}f(x) + V(x)f(x), \quad f \in \mathrm{Dom}\,(H_\alpha(t)), \tag{1.21}$$

where the domain $\mathrm{Dom}\,(H_\alpha(t))$ is given by

$$\mathrm{Dom}\,(H_\alpha(t)) := \tag{1.22}$$
$$\left\{ f \in W^{1,2}(\mathbb{R}) : \begin{array}{l} \frac{1}{M} f' \in W^{1,2}(\mathbb{R}) \\ (\frac{1}{2M} f')(a+0) - (\frac{1}{2M} f')(a-0) = e^{-\alpha t} f(a) \\ (\frac{1}{2M} f')(b+0) - (\frac{1}{2M} f')(b-0) = e^{-\alpha t} f(b) \end{array} \right\}.$$

After a rather standard analysis, one can prove the following convergence in the norm resolvent sense:

$$n - \lim_{t\to-\infty}(H_\alpha(t)-z)^{-1} = (H_D - z)^{-1} \tag{1.23}$$

and

$$n - \lim_{t\to+\infty}(H_\alpha(t)-z)^{-1} = (H - z)^{-1}, \tag{1.24}$$

$z \in \mathbb{C}\setminus\mathbb{R}$. Then we consider the quantum Liouville equation (details about the various topologies will follow later):

$$i\frac{\partial}{\partial t}\varrho_\alpha(t) = [H_\alpha(t), \varrho_\alpha(t)], \quad t\in\mathbb{R}, \tag{1.25}$$

for a fixed $\alpha > 0$ satisfying the initial condition

$$\text{s-}\lim_{t\to-\infty}\varrho_\alpha(t) = \varrho_D.$$

Having found a solution $\varrho_\alpha(t)$ we are interested in the ergodic limit

$$\varrho_\alpha = \lim_{T\to+\infty}\frac{1}{T}\int_0^T \varrho_\alpha(t)dt.$$

If we can verify that the limit ϱ_α exists and commutes with H, then ϱ_α is regarded as the desired NESS of the fully coupled system $\{\mathfrak{H}, H\}$. Inserting ϱ_α into the definition of the carrier density operator $\mathcal{N}_{\rho_\alpha}$ we complete the definition of the carrier density operator. Finally, the steady state ϱ_a allows to determine the corresponding distribution function $\{\tilde{\rho}_\alpha(\lambda)\}_{\lambda\in\mathbb{R}}$.

1.2 Outline of results

The precise formulation of our main result can be found in Theorem 3.6, and here we only describe its main features in words.

We need to introduce the incoming wave operator

$$W_- := \text{s-}\lim_{t\to-\infty} e^{itH}e^{-itH_D}P^{ac}(H_D) \tag{1.26}$$

where $P^{ac}(H_D)$ is the projection on the absolutely continuous subspace $\mathfrak{H}^{ac}(H_D)$ of H_D. We note that $\mathfrak{H}^{ac}(H_D) = L^2((-\infty,a])\oplus L^2([b,\infty))$. The wave operator exists and is complete, that is, W_- is an isometric operator acting from $\mathfrak{H}^{ac}(H_D)$ onto $\mathfrak{H}^{ac}(H)$ where $\mathfrak{H}^{ac}(H)$ is the absolutely continuous subspace of H (the range of $P^{ac}(H)$).

One not so surprising result, is that ϱ_α exists for all $\alpha > 0$. In fact, if we restrict ourselves to the subspace $\mathfrak{H}^{ac}(H)$, then we do not need to take the ergodic limit, since the usual strong limit exist. The surprising fact is that

$$\text{s-}\lim_{t\to\infty}\varrho_\alpha(t)P^{ac}(H) = \varrho_\alpha P^{ac}(H) = W_-\rho_D W_-^* P^{ac}(H), \tag{1.27}$$

which is *independent* of α.

The only α dependence can be found in $\varrho_\alpha P^d(H)$, where $P^d(H)$ is the projection on the subspace generated by the discrete eigenfunctions of H. But this part does not contribute to the stationary current as can be seen in Section 4. Here the ergodic limit is essential, because it kills off the oscillations produced by the interference between different eigenfunctions.

Note that the case $\alpha = \infty$ would describe the situation in which the coupling is suddenly made at $t = 0$ and then the system evolves freely with the dynamics generated by H (see [19], and the end of Section 3).

The case $\alpha \searrow 0$ would correspond to the adiabatic limit. Inspired by the physical literature which seems to claim that the adiabatic limit would take care of the above mentioned oscillations, we *conjecture* the following result for the transient current:

Conjecture 1.3

$$\lim_{\alpha \searrow 0} \limsup_{t \to \infty} \left| \mathrm{Tr}\{\varrho_\alpha(t) P^d(H)[H, \chi]\} \right| = 0,$$

where χ is any smoothed out characteristic function of one of the reservoirs.

Before ending this introduction, let us comment on some other physical aspects related to quantum transport problems. Many physics papers are dealing with transient currents and not only with the steady ones. More precisely, they investigate non-stationary electronic transport in noninteracting nanostructures driven by a finite bias and time-dependent signals applied at their contacts to the leads, while they allow the carriers to self-interact inside the quantum well (see for example [23, 24] and references therein).

A similar more abstract approach was used by Nier in [27]. An interesting open problem is to study the existence of NESS in the Cini (partition-free) approach [9, 12, 13, 14, 12]. Some nice results which are in the same spirit with ours have already been obtained in the physical literature [30, 31], even for systems which allow local self-interactions.

Now let us describe the organization of our paper.

Section 2 introduces all the necessary notation and presents an explicit description of a spectral representation of H_D and H.

Section 3 deals with the quantum Liouville equation, and contains the proof of our main result in Theorem 3.6.

In Section 4 we define the stationary current and derive the Landau-Lifschitz and Landauer-Büttiker formulas.

2 Technical preliminaries

2.1 The uncoupled system

Let us start by describing the uncoupled system, and begin with the left reservoir. The spectrum of H_a is absolutely continuous and $\sigma(H_a) = \sigma_{ac}(H_a) = [v_a, \infty)$. The operator is simple. The generalized eigenfunctions $\psi_a(\cdot, \lambda)$, $\lambda \in [v_a, \infty)$, of H_a are given by

$$\psi_a(x, \lambda) := \frac{\sin(2m_a q_a(\lambda)(x-a))}{\sqrt{\pi q_a(\lambda)}}, \quad x \in (-\infty, a], \quad \lambda \in [v_a, \infty)$$

where

$$q_a(\lambda) := \sqrt{\frac{\lambda - v_a}{2m_a}}.$$

The system of eigenfunctions $\{\psi_a(\cdot, \lambda)\}_{\lambda \in [v_a, \infty)}$ is orthonormal, that is, one has in distributional sense

$$\int_a^\infty dx\ \psi_a(x, \lambda)\overline{\psi_a(x, \mu)} = \delta(\lambda - \mu), \quad \lambda, \mu \in [v_a, \infty). \tag{2.1}$$

With the generalized eigenfunctions one associates the generalized Fourier transform $\Psi_a : L^2((-\infty, a]) \longrightarrow L^2([v_a, \infty))$ given by

$$(\Psi_a f)(\lambda) = \int_{-\infty}^a f(x)\overline{\psi_a(x, \lambda)}dx = \int_{-\infty}^a f(x)\psi_a(x, \lambda)dx,$$

$f \in L^2((-\infty, a])$. Using (2.1) a straightforward computation shows that the generalized Fourier is an isometry acting from $L^2((-\infty, a])$ onto $L^2([v_a, \infty))$. The inverse operator $\Psi_a^{-1} : L^2([v_a, \infty) \longrightarrow L^2(-\infty, a])$ admits the representation

$$(\Psi_a^{-1} f)(\lambda) = \int_{v_a}^\infty \psi_a(x, \lambda) f(\lambda) d\lambda = \int_{v_a}^\infty \frac{\sin(2m_a q_a(\lambda)(x-a))}{\sqrt{\pi q_a(\lambda)}} f(\lambda) d\lambda,$$

$f \in L^2([v_a, \infty))$. Since $\psi_a(\cdot, \lambda)$ are generalized eigenfunctions of H_a one easily verifies that

$$M_a = \Psi_a H_a \Psi_a^{-1} \quad \text{or} \quad H_a = \Psi_a^{-1} M_a \Psi_a$$

where M_a is the multiplication operator induced by the independent variable λ in $L^2([v_a, \infty))$ and defined by

$$\begin{aligned} (M_a f)(\lambda) &= \lambda f(\lambda), \\ f \in \mathrm{Dom}\,(M_a) &:= \{f \in L^2([v_a, \infty)) : \lambda f(\lambda) \in L^2([v_a, \infty))\}. \end{aligned}$$

This shows that $\{L^2([v_a, \infty)), M_a\}$ is a spectral representation of H_a. For the equilibrium sub-state $\varrho_a = \mathfrak{f}_a(H_a - \mu_a)$ one has the representation

$$\varrho_a = \Psi_a^{-1} M(\mathfrak{f}_a(\cdot - \mu_a))\Psi_a$$

where $M(\mathfrak{f}_a(\cdot - \mu_a))$ denotes the multiplication operator induced by the function $\mathfrak{f}_a(\cdot - \mu_a)$.

Let us continue with the closed quantum well. The operator $H_{\mathcal{I}}$ has purely discrete point spectrum $\{\xi_k\}_{k\in\mathbb{N}}$ with an accumulation point at $+\infty$. The eigenvalues are simple. The density operator $\varrho_{\mathcal{I}} = \mathfrak{f}_{\mathcal{I}}(H_{\mathcal{I}} - \mu_{\mathcal{I}})$ is trace class. One easily verifies that there is an isometric map $\Psi_{\mathcal{I}} : L^2((a,b)) \longrightarrow L^2(\mathbb{R}, \mathbb{C}, \nu_{\mathcal{I}})$, $d\nu_{\mathcal{I}}(\lambda) = \sum_{k=1}^{\infty} \delta(\lambda - \xi_k)d\lambda$, such that $\{L^2(\mathbb{R}, \mathbb{C}, \nu_{\mathcal{I}}), M_{\mathcal{I}}\}$ becomes a spectral representation of $H_{\mathcal{I}}$ where $M_{\mathcal{I}}$ denotes the multiplication operator in $L^2(\mathbb{R}, \mathbb{C}, \nu_{\mathcal{I}})$.

Finally, the right-hand reservoir. The spectrum of H_b is absolutely continuous and $\sigma(H_b) = \sigma_{ac}(H_b) = [v_b, \infty)$. The operator H_b is simple. The generalized eigenfunctions $\psi_b(\cdot, \lambda)$, $\lambda \in [v_b, \infty)$ are given by

$$\psi_b(x, \lambda) = \frac{\sin(2m_b q_b(\lambda)(x-b))}{\sqrt{\pi q_b(\lambda)}}, \quad x \in [b, \infty), \quad \lambda \in [v_b, \infty)$$

where

$$q_b(\lambda) = \sqrt{\frac{\lambda - v_b}{2m_b}}.$$

The generalized eigenfunctions $\{\psi_b(\cdot, \lambda)\}_{\lambda\in[v_b,\infty)}$ perform an orthonormal system and define a generalized Fourier transform $\Psi_b : L^2([b, \infty)) \longrightarrow L^2([v_b, \infty))$ by

$$(\Psi_b f)(\lambda) := \int_b^{\infty} f(x)\overline{\psi_b(x, \lambda)}dx = \int_b^{\infty} f(x)\psi_b(x, \lambda)dx,$$

$f \in L^2([b, \infty))$. The inverse Fourier transform $\Psi_b^{-1} : L^2([v_b, \infty)) \longrightarrow L^2([b, \infty))$ admits the representation

$$(\Psi_b^{-1} f)(x) = \int_{v_b}^{\infty} \psi_b(x, \lambda) f(\lambda)d\lambda = \int_{v_b}^{\infty} \frac{\sin(2m_b q_b(\lambda)(x-b))}{\sqrt{\pi q_b(\lambda)}} f(\lambda)d\lambda,$$

$f \in L^2([v_b, \infty))$. Denoting by M_b the multiplication operator induced by the independent variable λ in $L^2([v_b, \infty))$ we get

$$M_b = \Psi_b H_b \Psi_b^{-1} \quad \text{or} \quad H_b = \Psi_b^{-1} M_b \Psi_b$$

which shows that $\{L^2([v_b, \infty)), M_b\}$ is a spectral representation of H_b. The equilibrium sub-state $\varrho_b = \mathfrak{f}_b(H_b - \mu_b)$ is unitarily equivalent to the multiplication operator $M(\mathfrak{f}_b(\cdot - \mu_b))$ induced by the function $\mathfrak{f}_b(\cdot - \mu_b)$ in $L^2([v_b, \infty))$, that is,

$$\varrho_b = \Psi_b^{-1} M(\mathfrak{f}_b(\cdot - \mu_b))\Psi_b.$$

2.2 Spectral representation of the decoupled system

A straightforward computation shows that the direct sum $\Psi = \Psi_a \oplus \Psi_{\mathcal{I}} \oplus \Psi_b$ defines an isometric map acting from $L^2(\mathbb{R})$ onto $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu_D(\lambda))$, $d\nu_D(\lambda) = \sum_{k=1}^{\infty} \delta(\lambda -$

$\xi_k)d\lambda+\chi_{[v_b,\infty)}(\lambda)d\lambda$, such that H_D becomes unitarily equivalent to the multiplication operator M_D defined in $L^2(\mathbb{R},\mathfrak{h}(\lambda),\nu_D(\lambda))$ (see (1.5)). Here we slightly change the definition of $\mathfrak{h}(\lambda)$ such that it re-becomes $\mathbb{C}$ when λ hits an eigenvalue. This does not affect the absolutely continuous part.

Hence $\{L^2(\mathbb{R},\mathfrak{h}(\lambda),\nu_D(\lambda)),M_D\}$ is a spectral representation of H_D. Under the map Ψ the absolutely continuous part $H_D^{ac}=H_a\oplus H_b$ of H_D is unitarily equivalent to the multiplication operator M in $L^2(\mathbb{R},\mathfrak{h}(\lambda),\nu_D^{ac})$, $d\nu_D^{ac}(\lambda)=\chi_{[v_b,\infty)}(\lambda)d\lambda$. Therefore $\{L^2(\mathbb{R},\mathfrak{h}(\lambda),\nu_D^{ac}),M\}$ is a spectral representation of H_D^{ac}.

With respect to the spectral representation $\{L^2(\mathbb{R},\mathfrak{h}(\lambda),\nu_D),M\}$ the distribution function $\{\tilde\rho_D(\lambda)\}$ of the steady state ϱ_D is given by

$$\tilde\rho_D(\lambda):=\begin{cases}0, & \lambda\in\mathbb{R}\setminus\sigma(H_D)\\ \mathfrak{f}_{\mathcal{I}}(\lambda-\mu_{\mathcal{I}}), & \lambda\in\sigma_p(H_D)=\sigma(H_{\mathcal{I}})\\ \mathfrak{f}_b(\lambda-\mu_b), & \lambda\in[v_b,v_a)\setminus\sigma(H_{\mathcal{I}})\\ \begin{pmatrix}\mathfrak{f}_b(\lambda-\mu_b) & 0\\ 0 & \mathfrak{f}_a(\lambda-\mu_a)\end{pmatrix}, & \lambda\in[v_a,\infty)\setminus\sigma(H_{\mathcal{I}})\end{cases}$$

We note that $M(\tilde\rho_D)=\Psi\varrho_D\Psi^{-1}$.

2.3 The fully coupled system

The Hamiltonian H in (1.1) was investigated in detail in [6]. If $v_a\geq v_b$, then it turns out that the operator H has a finite simple point spectrum on $(-\infty,v_b)$, on $[v_b,v_a)$ the spectrum is absolutely continuous and simple, and on $[v_a,\infty)$ the spectrum is also absolutely continuous with multiplicity two.

Denoting by $\{\lambda_p\}_{p=1}^N$ the eigenvalues on $(-\infty,v_b)$, we have a corresponding finite sequence of L^2-eigenfunctions $\{\psi(x,\lambda_j)\}_{j=1}^N$.

Moreover, one can construct a set of generalized eigenfunctions $\phi_a(x,\lambda)$, $x\in\mathbb{R}$, $\lambda\in[v_a,\infty)$, and $\phi_b(x,\lambda)$, $x\in\mathbb{R}$, $\lambda\in[v_b,\infty)$ of H such that $\{\phi_b(\cdot,\lambda)\}_{\lambda\in[v_b,v_a)}$ and $\{\phi_b(\cdot,\lambda),\phi_a(\cdot,\lambda)\}_{\lambda\in[v_a,\infty)}$ generate a complete orthonormal systems of generalized eigenfunctions. More precisely:

$$\begin{aligned}\int_{\mathbb{R}}\phi_a(x,\lambda)\overline{\phi_a(x,\mu)}dx &= \delta(\lambda-\mu),\quad \lambda,\mu\in[v_a,\infty)\\ \int_{\mathbb{R}}\phi_b(x,\lambda)\overline{\phi_b(x,\mu)}dx &= \delta(\lambda-\mu),\quad \lambda,\mu\in[v_b,\infty)\\ \int_{\mathbb{R}}\phi_a(x,\lambda)\overline{\phi_b(x,\mu)}dx &= 0,\quad \lambda,\mu\in[v_a,\infty),\end{aligned}$$

see [6]. The existence of generalized eigenfunctions is shown by constructing solutions $\widetilde{\phi}_a(x,\lambda)$ and $\widetilde{\phi}_b(x,\lambda)$ of the ordinary differential equation

$$-\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}\widetilde{\phi}_p(x,\lambda)+v(x)\widetilde{\phi}_p(x,\lambda)=\lambda\widetilde{\phi}_p(x,\lambda),$$

$x \in \mathbb{R}$, $\lambda \in [v_b, \infty)$, $p = a, b$, obeying

$$\widetilde{\phi}_a(x,\lambda) = \begin{cases} e^{i2m_a q_a(\lambda)(x-a)} + S_{aa}(\lambda) e^{-i2m_a q_a(\lambda)(x-a)} & x \in (-\infty, a] \\ S_{ba}(\lambda) e^{i2m_b q_b(\lambda)(x-b)} & x \in [b, \infty), \end{cases}$$

$\lambda \in [v_a, \infty)$, and

$$\widetilde{\phi}_b(x,\lambda) = \begin{cases} S_{ab}(\lambda) e^{-i2m_a q_a(\lambda)(x-a)} & x \in (-\infty, a] \\ e^{-i2m_b q_b(\lambda)(x-b)} + S_{bb}(\lambda) e^{i2m_b q_b(\lambda)(x-b)} & x \in [b, \infty), \end{cases}$$

$\lambda \in [v_b, \infty)$. The coefficients $S_{aa}(\lambda)$ and $S_{bb}(\lambda)$ are called reflection coefficients while $S_{ba}(\lambda)$ and $S_{ab}(\lambda)$ are called transmission coefficients. The solutions $\widetilde{\phi}_a(\lambda)$ and $\widetilde{\phi}_b(\lambda)$ define the normalized generalized eigenfunctions of H by

$$\phi_b(x,\lambda) := \frac{1}{4\pi q_b(\lambda)} \widetilde{\phi}_b(x,\lambda), \quad x \in \mathbb{R}, \quad \lambda \in [v_b, \infty),$$
$$\phi_a(x,\lambda) := \frac{1}{4\pi q_a(\lambda)} \widetilde{\phi}_a(x,\lambda), \quad x \in \mathbb{R}, \quad \lambda \in [v_a, \infty).$$

Having the existence of the generalized eigenfunctions one introduces the generalized Fourier transform $\Phi : L^2(\mathbb{R}) \longrightarrow L^2(\mathfrak{h}(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$ by

$$(\Phi f)(\lambda) := \int_{\mathbb{R}} f(x) \overline{\vec{\phi}(x,\lambda)} dx, \quad f \in L^2(\mathbb{R}), \quad \lambda \in \sigma(H), \tag{2.2}$$

where

$$\vec{\phi}(x,\lambda) := \begin{cases} \phi(x,\lambda_j) & \lambda \in \sigma_p(H), \quad x \in \mathbb{R} \\ \phi_b(x,\lambda) & \lambda \in [v_b, v_a), \quad x \in \mathbb{R} \\ \begin{pmatrix} \phi_b(x,\lambda) \\ \phi_a(x,\lambda) \end{pmatrix} & \lambda \in [v_b, \infty), \quad x \in \mathbb{R}, \end{cases} \tag{2.3}$$

see [6]. The inverse generalized Fourier transform $\Phi^{-1} : L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu) \longrightarrow L^2(\mathbb{R})$ is given by

$$(\Phi^{-1} g) = \int_{\mathbb{R}} \langle g(\lambda), \overline{\vec{\phi}(x,\lambda)} \rangle_{\mathfrak{h}(\lambda)} d\nu(\lambda), \tag{2.4}$$

$x \in \mathbb{R}$, $g \in L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$ where $\langle \cdot, \cdot \rangle_{\mathfrak{h}(\lambda)}$ is the scalar product in $\mathfrak{h}(\lambda)$. Since Φ is an isometry action from $L^2(\mathbb{R})$ onto $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$ and

$$M = \Phi H \Phi^{-1}$$

holds where M is the multiplication operator induced by the independent variable in $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$ one gets that $\{L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu), M\}$ is a spectral representation of H.

Under Φ the absolutely continuous part H^{ac} becomes unitarily equivalent to the multiplication operator M in $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu^{ac})$, $d\nu^{ac} = \chi_{[v_b,\infty)} d\lambda$. Hence $\{L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu^{ac}), M\}$ is a spectral representation of H^{ac}, as it was for H_D^{ac}.

2.4 The incoming wave operator

We have already mentioned that W_- as defined in (1.26) exists and is complete [33]. We will need in Section 4 the expression of the "rotated" wave operator $\Phi W_- \Psi^{-1}$ which acts from $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu^{ac})$ onto itself. By direct (but tedious) computations one can show that $\widehat{W}_- := \Phi W_- \Psi^{-1}$ acts as a multiplication operator, which means that there is a family $\{\widetilde{W}_-(\lambda)\}_{\lambda\in\mathbb{R}}$ of isometries acting from $\mathfrak{h}(\lambda)$ onto $\mathfrak{h}(\lambda)$ such that

$$(\widehat{W}_- f)(\lambda) = \widetilde{W}_-(\lambda) f(\lambda), \quad f \in L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu^{ac}).$$

The family $\{\widetilde{W}_-(\lambda)\}_{\lambda\in\mathbb{R}}$ is called the incoming wave matrix and can be explicitly calculated. One gets

$$\widetilde{W}_-(\lambda) = \begin{cases} i & \lambda \in [v_b, v_a] \\ \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} & \lambda \in (v_a, \infty). \end{cases} \tag{2.5}$$

Note that another possible approach to the spectral problem (and completely different) would be to construct generalized eigenfunctions for H out of those of H_D by using the unitarity of W_- between their subspaces of absolute continuity and the formal intertwining identity $\phi_p(\cdot, \lambda) := W_- \psi_p(\cdot, \lambda)$. In this case $\widetilde{W}_-(\lambda)$ would always equal the identity matrix.

3 The quantum Liouville equation

The time dependent operators $H_\alpha(t)$ from (1.20) are defined by the sesquilinear forms $\mathfrak{h}_\alpha[t](\cdot,\cdot)$,

$$\mathfrak{h}_\alpha[t](f,g) = \tag{3.1}$$
$$\int_{\mathbb{R}} \left\{ f'(x)\overline{g'(x)} + V(x) f(x) \overline{g(x)} \right\} dx + e^{-\alpha t} f(a)\overline{g(a)} + e^{-\alpha t} f(b)\overline{g(b)},$$

$f, g \in \mathrm{Dom}\,(\mathfrak{h}_a[t]) := W^{1,2}(\mathbb{R})$, $t \in \mathbb{R}$. Obviously, we have $H_\alpha(t) + \tau \geq I$, $\tau := \|V\|_{L^\infty(\mathbb{R})} + 1$. For each $t \in \mathbb{R}$ the operator $H_\alpha(t)$ can be regarded as a bounded operator acting from $W^{1,2}(\mathbb{R})$ into $W^{-1,2}(\mathbb{R})$. Classical Sobolev embedding results ensure that $(H_\alpha(t) + \tau)^{-1/2}$ maps $L^2(\mathbb{R})$ into continuous functions, and it has an integral kernel $G(x, x'; \tau)$ with the property that $G(\cdot, x'; \tau) \in L^2(\mathbb{R})$ for every fixed x'.

Let us introduce the operators $B_a : L^2(\mathbb{R}) \longrightarrow \mathbb{C}$ and $B_b : L^2(\mathbb{R}) \longrightarrow \mathbb{C}$ defined by:

$$(B_a f) := [(H_\alpha(t) + \tau)^{-1/2} f](a) = \tag{3.2}$$
$$\int_{\mathbb{R}} G(a, x; \tau) f(x) dx, \qquad (B_a^* c)(x) = G(x, a; \tau),$$

and similarly for B_b. The operators $B_a^*B_a$ and $B_b^*B_b$ are bounded in $L^2(\mathbb{R})$ and correspond to the sesquilinear forms

$$\mathfrak{b}_a[t](f,g) := ((H_\alpha(t)+\tau)^{-1/2}f)(a)\overline{((H_\alpha(t)+\tau)^{-1/2}g)(a)},$$

$f, g \in \mathrm{Dom}\,(\mathfrak{b}_a[t]) = L^2(\mathbb{R})$, and

$$\mathfrak{b}_b[t](f,g) := ((H_\alpha(t)+\tau)^{-1/2}f)(b)\overline{((H_\alpha(t)+\tau)^{-1/2}g)(b)},$$

$f, g \in \mathrm{Dom}\,(\mathfrak{b}_b[t]) = L^2(\mathbb{R})$, respectively. We define the rank two operator

$$\begin{aligned} B := B_a^*B_a + B_b^*B_b = \\ G(\cdot,a;\tau)G(a,\cdot;\tau) + G(\cdot,b;\tau)G(b,\cdot;\tau) : L^2(\mathbb{R}) \longrightarrow L^2(\mathbb{R}). \end{aligned} \tag{3.3}$$

The resolvent $(H_\alpha(t)+\tau)^{-1}$ admits the representation

$$(H_\alpha(t)+\tau)^{-1} = (H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-1}(H+\tau)^{-1/2}, \quad t\in\mathbb{R}, \quad \alpha>0. \tag{3.4}$$

3.1 The unitary evolution

Let us consider a weakly differentiable map $\mathbb{R} \ni t \mapsto u(t) \in W^{1,2}(\mathbb{R})$. We are interested in the evolution equation

$$i\frac{\partial}{\partial t}u(t) = H_\alpha(t)u(t), \quad t\in\mathbb{R}, \quad \alpha>0. \tag{3.5}$$

where $H_\alpha(t)$ is regarded as a bounded operator acting from $W^{1,2}(\mathbb{R})$ into $W^{-1,2}(\mathbb{R})$.

By Theorem 6.1 of [25] with evolution equation (3.5) one can associate a unique unitary solution operator or propagator $\{U(t,s)\}_{(t,s)\in\mathbb{R}\times\mathbb{R}}$ leaving invariant the Hilbert space $W^{1,2}(\mathbb{R})$. By Theorem 8.1 of [21] we find that for $x, y \in W^{1,2}(\mathbb{R})$ the sesquilinear form $(U(t,s)x,y)$ is continuously differentiable with respect $t\in\mathbb{R}$ and $s\in\mathbb{R}$ such that

$$\frac{\partial}{\partial t}(U(t,s)x,y) = -i(H_\alpha(t)U(t,s)x,y), \quad x,y\in W^{1,2}(\mathbb{R}), \tag{3.6}$$

$$\frac{\partial}{\partial s}(U(t,s)x,y) = i(H_\alpha(s)x,U(s,t)y), \quad x,y\in W^{1,2}(\mathbb{R}). \tag{3.7}$$

3.2 Quantum Liouville equation

We note that

$$\varrho_\alpha(t) := U(t,s)\varrho_\alpha(s)U(s,t), \quad t,s\in\mathbb{R}, \tag{3.8}$$

seen as a map from $W^{1,2}(\mathbb{R})$ into $W^{-1,2}(\mathbb{R})$ is differentiable and solves the quantum Liouville equation (1.25) satisfying the initial condition $\varrho_\alpha(t)|_{t=s} = \varrho_\alpha(s)$, provided $\varrho_\alpha(s)$ leaves $W^{1,2}(\mathbb{R})$ invariant. Indeed, using (3.6) and (3.7) we find

$$\begin{aligned} &\frac{\partial}{\partial t}(\varrho_\alpha(s)U(s,t)x,U(s,t)y) = \\ &\quad i(U(s,t)H_\alpha(t)x,\varrho_\alpha(s)U(s,t)y) - i((\varrho_\alpha(s)U(s,t)x,U(s,t)H_\alpha(t)y) = \\ &\quad i(H_\alpha(t)x,\varrho_\alpha(t)y) - i(\varrho_\alpha(t)x,H_\alpha(t)y), \end{aligned}$$

$x, y \in W^{1,2}(\mathbb{R})$, which yields

$$i\frac{\partial}{\partial t}(\varrho_\alpha(t)x, y) = (\varrho_\alpha(t)x, H_\alpha(t)y) - (H_\alpha(t)x, \varrho_\alpha(t)y),$$

$x, y \in W^{1,2}(\mathbb{R})$, $t, s \in \mathbb{R}$.

3.3 Time dependent scattering

We set $U(t) := U(t, 0)$, $t \in \mathbb{R}$ and consider the wave operators

$$\Omega_- := \text{s-}\lim_{t\to-\infty} U(t)^* e^{-itH_D}$$

and

$$\Omega_+ := \text{s-}\lim_{t\to+\infty} U(t)^* e^{-itH}.$$

Proposition 3.1 *Let H_D and $H_\alpha(t)$, $t \in \mathbb{R}$, $\alpha > 0$, be given by* (1.8)-(1.16) *and* (1.21)-(1.22)*, respectively. Then the wave operator Ω_- and the limit*

$$R_- := \text{s-}\lim_{t\to-\infty} U(t)^*(H_D + \tau)^{-1}U(t) \tag{3.9}$$

exist. Moreover,

$$\text{Ran}(\Omega_-)^\perp = \text{Ker}(R_-). \tag{3.10}$$

Proof. We start with (3.9). Let us introduce the time-dependent identification operator

$$J_D(t) := (H_\alpha(t) + \tau)^{-1}(H_D + \tau)^{-1}, \quad t \in \mathbb{R}.$$

We have

$$\begin{aligned}&\frac{d}{dt}U(t)^* J_D(t)e^{-itH_D}f = \\ &\quad iU(t)^*\left((H_D + \tau)^{-1} - (H_\alpha(t) + \tau)^{-1}\right)e^{-itH_D}f + U(t)^*\dot{J}_D(t)e^{-itH}f\end{aligned} \tag{3.11}$$

for $f \in \mathfrak{H}$ where $\dot{J}_D := \frac{d}{dt}J_D(t)$. Hence we get

$$\begin{aligned}&U(t)J_D(t)e^{-itH_D}f - U(s)^*J_D(s)e^{-isH_D}f = \\ &\quad i\int_s^t U(s)^*\left((H_D + \tau)^{-1} - (H_\alpha(r) + \tau)^{-1}\right)e^{-irH_D}f dr + \\ &\quad \int_0^t U(r)^*\dot{J}_D(r)e^{-irH_D}f ds.\end{aligned} \tag{3.12}$$

Using (3.4) we find

$$\begin{aligned}&(H_\alpha(t) + \tau)^{-1} = (H + \tau)^{-1/2}Q_B(H + \tau)^{-1/2} + \\ &\quad e^{\alpha t}(H + \tau)^{-1/2}Q_B^\perp(e^{\alpha t} + B)^{-1}Q_B^\perp(H + \tau)^{-1/2}\end{aligned} \tag{3.13}$$

where Q_B is the orthogonal projection onto the subspace $\mathrm{Ker}(B)$. Note that $Q_B^\perp$ has rank 2. Taking into account (1.23) we get the representation

$$(H_D+\tau)^{-1} = (H+\tau)^{-1/2} Q_B (H+\tau)^{-1/2}. \tag{3.14}$$

By (3.13) and (3.14) we obtain

$$\begin{aligned}(H_D+\tau)^{-1} - (H_\alpha(t)+\tau)^{-1} = \\ -e^{\alpha t}(H+\tau)^{-1/2} Q_B^\perp (e^{\alpha t}+B)^{-1} Q_B^\perp (H+\tau)^{-1/2}.\end{aligned} \tag{3.15}$$

Since B is positive and invertible on $\mathrm{Ker}(B)^\perp$ we get the estimate

$$\|(H_D+\tau)^{-1} - (H_\alpha(t)+\tau)^{-1}\| \le e^{\alpha t}\|Q_B^\perp B^{-1} Q_B^\perp\|, \quad t\in\mathbb{R}, \quad \alpha>0. \tag{3.16}$$

Using again (3.13) we have

$$\dot J_D(t) = \alpha e^{\alpha t}(H+\tau)^{-1/2} Q_B^\perp (e^{\alpha t}+B)^{-2} B Q_B^\perp (H+\tau)^{-1/2}(H_D+\tau)^{-1}. \tag{3.17}$$

This gives the estimate

$$\|\dot J_D(t)\| \le \alpha e^{\alpha t}\|Q_B^\perp B^{-1} Q_B^\perp\|. \tag{3.18}$$

Using (3.12), (3.16) and (3.18) we prove the existence of the limit

$$\widehat\Omega_- := \text{s-}\lim_{t\to-\infty} U(t)^* J_D(t) e^{-itH_D}.$$

In fact, the convergence is in the operator norm:

$$\lim_{t\to-\infty} \|\widehat\Omega_- - U(t)^* J_D(t) e^{-itH_D}\| = 0. \tag{3.19}$$

Using the identity

$$\begin{aligned}U(t)^* J_D(t) e^{-itH_D} - U(t)^* e^{-itH_D}(H_D+\tau)^{-2} \\ = U(t)^*((H_\alpha(t)+\tau)^{-1} - (H_D+\tau)^{-1}) e^{-itH_D}(H_D+\tau)^{-1}\end{aligned}$$

and (3.16) we get the estimate

$$\|U(t)^* J_D(t) e^{-itH_D} - U(t)^* e^{-itH_D}(H_D+\tau)^{-2}\| \le e^{\alpha t}\|Q_B^\perp B^{-1} Q_B^\perp\|, \tag{3.20}$$

which yields

$$\lim_{t\to-\infty} \|\widehat\Omega_- - U(t)^* e^{-itH_D}(H_D+\tau)^{-2}\| = 0, \tag{3.21}$$

for all $t\in\mathbb{R}$, $\alpha>0$. Since the wave operator $\widehat\Omega_-$ exists we get the existence of

$$\text{s-}\lim_{t\to-\infty} U(t)^* e^{-itH_D}(H_D+\tau)^{-2}.$$

Using that $\mathrm{Ran}\,((H_D+\tau)^{-2})$ is dense in $\mathfrak{H}$, we prove the existence of Ω_-. In particular, this proves that Ω_- is isometric, i.e $\Omega_-^*\Omega_- = I$.

Now let us prove that the operator in (3.9) exists. Note that the norm convergence in (3.19) yields the same property for adjoints:

$$\lim_{t\to-\infty}\|\widehat{\Omega}_-^* - e^{itH_D}J_D(t)^*U(t)\| = 0.$$

In particular

$$\widehat{\Omega}_-^* = \text{s-}\lim_{t\to-\infty} e^{itH_D}J_D(t)^*U(t).$$

In the quadratic form sense we get

$$\frac{d}{dt}U(t)^*(H_\alpha(t)+\tau)^{-1}U(t)f = U(t)^*\left\{\frac{d}{dt}(H_\alpha(t)+\tau)^{-1}\right\}U(t)f$$

$f\in\mathfrak{H}$, $t\in\mathbb{R}$, $\alpha>0$. Hence

$$\begin{aligned}U(t)^*(H_\alpha(t)+\tau)^{-1}U(t)f - U(s)^*(H_\alpha(t)+\tau)^{-1}U(s)f\\ = \int_s^t dr\; U(r)^*\left\{\frac{d}{dr}(H_\alpha(r)+\tau)^{-1}\right\}U(r)f\end{aligned}$$

$f\in\mathfrak{H}$, $t,s\in\mathbb{R}$, $\alpha>0$. By (3.4) we get

$$\frac{d}{dt}(H_\alpha(t)+\tau)^{-1} = \alpha e^{-\alpha t}(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-1/2}$$

which gives the estimate

$$\left\|\frac{d}{dt}(H_\alpha(t)+\tau)^{-1}\right\| \le \alpha e^{\alpha t}\|Q_B^\perp B^{-1}Q_B^\perp\|. \tag{3.22}$$

Hence R_- exists, and we even have convergence in operator norm:

$$\lim_{t\to-\infty}\|R_- - U(t)^*(H_\alpha(t)+\tau)^{-1}U(t)^*\| = 0.$$

Taking into account the estimate (3.16) we find

$$\lim_{t\to-\infty}\|R_- - U(t)^*(H_D+\tau)^{-1}U(t)^*\| = 0. \tag{3.23}$$

In particular we have

$$\begin{aligned}\lim_{t\to-\infty}\|R_-^2 - U(t)^*(H_\alpha(t)+\tau)^{-2}U(t)^*\|\\ = \lim_{t\to-\infty}\|R_-^2 - U(t)^*(H_D+\tau)^{-2}U(t)^*\| = 0.\end{aligned}$$

Using the identity

$$J_D(t)^* = \left((H_D+\tau)^{-1} - (H_\alpha(t)+\tau)^{-1}\right)(H_\alpha(t)+\tau)^{-1} + (H_\alpha(t)+\tau)^{-2}$$

and taking into account the estimate (3.16) we obtain

$$\lim_{t\to-\infty}\|R_-^2 - U(t)^*J_D(t)^*U(t)\| = 0.$$

Hence we find

$$\begin{aligned}\widehat{\Omega}_-^* &= \text{s-}\lim_{t\to-\infty} e^{itH_D} J_D(t)^* U(t) \\ &= \text{s-}\lim_{t\to-\infty} e^{itH_D} U(t) U(t)^* J_D(t)^* U(t) = \text{s-}\lim_{t\to-\infty} e^{itH_D} U(t) R_-^2\end{aligned} \tag{3.24}$$

which shows in particular that the limit $\lim_{t\to-\infty} e^{itH_D}U(t)f$ exist for elements $f \in \overline{\text{Ran}\,(R_-)}$. More precisely:

$$\lim_{t\to-\infty} e^{itH_D} U(t) R_- f = \Omega_-^* R_- f \tag{3.25}$$

for all f.

We are now ready to prove (3.10). Assume that $f \perp \text{Ran}\,(\Omega_-)$. Then using the definitions, the unitarity of $U(t)^*$, and (3.23) we obtain:

$$\begin{aligned}0 &= (f, \Omega_-(H_D+\tau)^{-1} g) \\ &= \lim_{t\to-\infty} (U(t)^*(H_D+\tau)^{-1} U(t) f, U(t)^* e^{-itH_D} g) = (R_- f, \Omega_- g)\end{aligned}$$

for $g \in \mathfrak{H}$. Hence $f \perp \text{Ran}\,(\Omega_-)$ implies $R_- f \perp \text{Ran}\,(\Omega_-) = \text{Ker}(\Omega_-^*)$. Thus $\Omega_-^* R_- f = 0$. Using (3.25):

$$0 = \lim_{t\to-\infty} \|e^{itH_D} U(t) R_- f\| = \|R_- f\|,$$

thus $f \in \text{Ker}(R_-)$. We have thus shown that $\text{Ran}\,(\Omega_-)^\perp \subset \text{Ker}(R_-)$. Conversely, choose $f \in \text{Ker}(R_-)$. We have (use (3.23)):

$$\begin{aligned}(f, \Omega_-(H_D+\tau)^{-1} g) &= \lim_{t\to-\infty} (f, U(t)^* e^{-itH_D} (H_D+\tau)^{-1} g) \\ &= \lim_{t\to-\infty} (U(t)^*(H_D+\tau)^{-1} U(t) f, U(t)^* e^{-itH_D} g) = (R_- f, \Omega_- g) = 0,\end{aligned}$$

for all g. Thus $\Omega_-^* f$ is orthogonal on a dense set (domain of H_D), thus equals zero. Therefore $\text{Ker}(R_-) \subset \text{Ran}\,(\Omega_-)^\perp$ and (3.10) is proved. □

Remark 3.2 Note that Ω_- is unitary if $\text{Ker}(R_-) = \emptyset$.

Proposition 3.3 *Let H and $H_\alpha(t)$, $t \in \mathbb{R}$, $\alpha > 0$, be given by* (1.1)-(1.4) *and* (1.21)-(1.22)*, respectively. Then the wave operator Ω_+ exists and is unitary.*

Proof. We introduce the identification operator

$$J(t) := (H_\alpha(t)+\tau)^{-1}(H+\tau)^{-1}. \quad t \in \mathbb{R}.$$

In the quadratic form sense we get that

$$\begin{aligned}&\frac{d}{dt} U(t)^* J(t) e^{-itH} f = \\ &\quad iU(t)^*((H+\tau)^{-1} - (H_\alpha(t)+\tau)^{-1}) e^{-itH} f + U(t)^* \dot{J}(t) e^{-itH} f,\end{aligned} \tag{3.26}$$

$t \in \mathbb{R}$, where

$$\dot{J}(t) := \frac{d}{dt} J(t).$$

Taking into account (3.4) we find

$$(H+\tau)^{-1} - (H_\alpha(t)+\tau)^{-1} = e^{-\alpha t}(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-1}B(H+\tau)^{-1/2}, \quad (3.27)$$

$t \in \mathbb{R}$. Hence we have the estimate

$$\|(H+\tau)^{-1} - (H_\alpha(t)+\tau)^{-1}\| \leq e^{-\alpha t}\|B\|, \quad t \in \mathbb{R}. \quad (3.28)$$

Moreover, we get

$$\begin{aligned} \dot{J}(t) &= \frac{d}{dr}(H_\alpha(t)+\tau)^{-1}(H+\tau)^{-1} \quad (3.29) \\ &= \alpha e^{-\alpha t}(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-3/2} \end{aligned}$$

which yields the estimate

$$\left\| \dot{J}(t) \right\| \leq \alpha e^{-\alpha t}\|B\|, \quad t \in \mathbb{R}.$$

Hence the strong limit

$$\widehat{\Omega}_+ := \text{s-}\lim_{t\to+\infty} U(t)^* J(t) e^{-itH}$$

exists. Moreover, the convergence is also true in operator norm:

$$\lim_{t\to+\infty} \|\widehat{\Omega}_+ - U(t)^* J(t) e^{-itH}\| = 0. \quad (3.30)$$

Using the identity

$$\begin{aligned} &U(t)^* J(t) e^{-itH} - U(t)^* e^{-itH}(H+\tau)^{-2} = \quad (3.31) \\ &\quad U(t)^* \left((H_\alpha(t)+\tau)^{-1} - (H+\tau)^{-1} \right) e^{-itH}(H+\tau)^{-1} \end{aligned}$$

and taking into account the estimate (3.28) we obtain

$$\lim_{t\to+\infty} \|\widehat{\Omega}_+ - U(t)^* e^{-itH}(H+\tau)^{-2}\| = 0. \quad (3.32)$$

Hence Ω_+ exists on a dense domain and is isometric, i.e. $\Omega_+^*\Omega_+ = I$.

Let us now prove that Ω_+ is unitary. Since (3.30) holds also true for adjoints we find

$$\lim_{t\to+\infty} \|\widehat{\Omega}_+^* - e^{itH} J(t) U(t)\| = 0. \quad (3.33)$$

Hence, we have the representation

$$\widehat{\Omega}_+^* = \text{s-}\lim_{t\to+\infty} e^{itH} J(t) U(t). \quad (3.34)$$

Furthermore, in the quadratic form sense we have

$$\frac{d}{dt}U(t)^*(H_\alpha(t)+\tau)^{-1}U(t) = U(t)^*\left\{\frac{d}{dt}(H_\alpha(t)+\tau)^{-1}\right\}U(t) = \alpha e^{-\alpha t}U(t)^*(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-1/2}U(t).$$

Hence we get

$$U(t)^*(H_\alpha(t)+\tau)^{-1}U(t) = (H_\alpha(0)+\tau)^{-1} + \alpha\int_0^t e^{-\alpha t}U(t)^*(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-1/2}U(t)dt. \tag{3.35}$$

Using the estimate

$$\left\|U(t)^*(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-1/2}U(t)\right\| \le \|B\|, \quad t\in\mathbb{R},$$

we find that the following weak integral exists and defines a bounded operator:

$$\alpha\int_0^\infty dt\, e^{-\alpha t}U(t)^*(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-1/2}U(t). \tag{3.36}$$

Moreover, by the Cook argument it also implies the existence of the limit

$$R_+ := \text{s-}\lim_{t\to+\infty} U(t)^*(H_\alpha(t)+\tau)^{-1}U(t).$$

In fact, the convergence takes place in operator norm:

$$\lim_{t\to+\infty}\|R_+ - U(t)^*(H_\alpha(t)+\tau)^{-1}U(t)\| = 0.$$

Taking into account the estimate (3.28) we obtain

$$\lim_{t\to+\infty}\|R_+ - U(t)^*(H+\tau)^{-1}U(t)\| = 0.$$

which yields

$$\lim_{t\to+\infty}\|R_+^2 - U(t)^*J(t)U(t)\| = 0.$$

By (3.33) we get

$$\lim_{t\to+\infty}\|\widehat{\Omega}_+^* - e^{itH}U(t)R_+^2\| = 0$$

which shows the existence of $\Omega_+^* f = \text{s-lim}_{t\to+\infty} e^{itH}U(t)f$ for $f\in\overline{\text{Ran}\,(R_+)}$. Now in order to prove the unitarity of Ω_+ it is enough to show that $\text{Ran}\,(R_+)$ is dense in $\mathfrak{H}$. Let us do that.

From (3.35) we obtain

$$R_+ = (H_\alpha(0)+\tau)^{-1} + \alpha\int_0^\infty dt\, e^{-\alpha t}U(t)^*(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-2}B(H+\tau)^{-1/2}U(t),$$

which by the positivity of the integral it gives $0 \leq (H_\alpha(0)+\tau)^{-1} \leq R_+$. Hence

$$\mathrm{Ker}(R_+^{1/2}) \subseteq \mathrm{Ker}((H_\alpha(0)+\tau)^{-1/2}),$$

thus

$$\mathrm{Ran}\,(R_+^{1/2})^\perp \subseteq \mathrm{Ran}\,((H_\alpha(0)+\tau)^{-1/2})^\perp = \emptyset.$$

Thus we get that $\mathrm{Ran}\,(R_+^{1/2})$ is dense in $\mathfrak{H}$ which yields that $\mathrm{Ran}\,(R_+^2)$ is dense in $\mathfrak{H}$. Therefore we have the representation $\Omega_+^* = \text{s-lim}_{t\to+\infty} e^{itH}U(t)$ which proves that Ω_+ is unitary. □

3.4 Time-dependent density operator

Now we are ready to write down a solution to our Liouville equation (1.25) which also obeys the initial condition at $t=-\infty$. Let us introduce the notation:

$$\varrho_\alpha(0) := \Omega_- \varrho_D \Omega_-^*$$

which defines a non-negative self-adjoint operator. Here ϱ_D is given by (1.17)-(1.19). In accordance with (3.8), the time evolution of $\varrho_\alpha(0)$ is given by

$$\varrho_\alpha(t) = U(t)\varrho_\alpha(0)U(t)^* = U(t)\Omega_-\varrho_D\Omega_-^*U(t)^*, \quad t\in\mathbb{R}, \tag{3.37}$$

where we have used the notation $U(t) := U(t,0)$ and the relation $U(0,t) = U(t)^*$, $t\in\mathbb{R}$. We now show that the initial condition is fulfilled.

Proposition 3.4 *Let H_D and $H_\alpha(t)$, $t\in\mathbb{R}$, $\alpha>0$, be given by* (1.8)-(1.16) *and* (1.21)-(1.22)*, respectively. If ϱ_D is a steady state for the system $\{\mathfrak{H}, H_D\}$ such that the operator $\widehat{\varrho}_D := (H_D+\tau)^4\varrho_D$ is bounded, then*

$$\lim_{t\to-\infty} \|\varrho_D - \varrho_\alpha(t)\| = 0. \tag{3.38}$$

Proof. We write the identity:

$$U(t)\Omega_-\varrho_D\Omega_-^*U(t)^* = U(t)\Omega_-(H_D+\tau)^{-2}\widehat{\varrho}_D(H_D+\tau)^{-2}\Omega_-^*U(t)^*, \tag{3.39}$$

$t\in\mathbb{R}$. Taking into account (3.21) we find

$$U(t)\Omega_-\varrho_D\Omega_-^*U(t)^* = U(t)\widehat{\Omega}_-\widehat{\varrho}_D\widehat{\Omega}_-^*U(t)^*. \tag{3.40}$$

From (3.19) we get

$$\begin{aligned}\lim_{t\to-\infty} \|U(t)\widehat{\Omega}_-\widehat{\varrho}_D\widehat{\Omega}_-^*U(t)^* - J_D(t)e^{-itH_D}\widehat{\varrho}_D e^{itH_D}J_D(t)^*\| \\ = \lim_{t\to-\infty}\|U(t)\widehat{\Omega}_-\widehat{\varrho}_D\widehat{\Omega}_-^*U(t)^* - J_D(t)\widehat{\varrho}_D J_D(t)^*\| = 0.\end{aligned} \tag{3.41}$$

Using (3.16) we get

$$\begin{aligned}\lim_{t\to-\infty} \|J_D(t)\widehat{\varrho}_D J_D(t)^* - (H_D+\tau)^{-2}\widehat{\varrho}_D(H_D+\tau)^{-2}\| \\ = \lim_{t\to-\infty}\|J_D(t)\widehat{\varrho}_D J_D(t)^* - \varrho_D\| = 0\end{aligned} \tag{3.42}$$

Taking into account (3.39)-(3.42) we prove (3.38). □

3.5 Large time behavior on the space of absolute continuity

We now are ready to prove the result announced in (1.27).

Proposition 3.5 *Let H and $H_\alpha(t)$, $t \in \mathbb{R}$, $\alpha > 0$, be given by* (1.1)-(1.4) *and* (1.21)-(1.22)*, respectively. Let W_- be the incoming wave operator as defined in* (1.26)*. If ϱ_D is a steady state for the system $\{\mathfrak{H}, H_D\}$ such that the operator $\widehat{\varrho}_D := (H_D + \tau)^4 \varrho_D$ is bounded, then*

$$\text{s-}\lim_{t\to+\infty} \varrho_\alpha(t) P^{ac}(H) = W_- \varrho_D W_-^*. \tag{3.43}$$

Proof.

Let us assume that the following three technical results hold true:

$$\text{s-}\lim_{t\to+\infty} (U(t)^* - e^{itH}) P^{ac}(H) = 0, \tag{3.44}$$

$$(H_D + \tau)^{-2}(\Omega_-^* - I) \quad \text{is} \quad \text{compact}, \tag{3.45}$$

and

$$\text{s-}\lim_{t\to+\infty} (H_D + \tau)^{-2}(\Omega_-^* - I) e^{itH} P^{ac}(H) = 0. \tag{3.46}$$

We will first use these estimates in order to prove the proposition, and then we will give their own proof.

We write the identity:

$$\begin{aligned}
&U(t)\varrho_\alpha(t)U(t)^* P^{ac}(H) \\
&\quad = U(t)\Omega_-(H_D+\tau)^{-2}\widehat{\varrho}_D(H_D+\tau)^{-2}\Omega_-^* U(t)^* P^{ac}(H) \\
&\quad = U(t)\Omega_-(H_D+\tau)^{-2}\widehat{\varrho}_D(H_D+\tau)^{-2}\Omega_-^* (U(t)^* - e^{itH}) P^{ac}(H) \\
&\quad + U(t)\Omega_-(H_D+\tau)^{-2}\widehat{\varrho}_D(H_D+\tau)^{-2}(\Omega_-^* - I) e^{itH} P^{ac}(H) \\
&\quad + U(t)\Omega_-(H_D+\tau)^{-2} e^{itH_D}\widehat{\varrho}_D(H_D+\tau)^{-2} e^{-itH_D} e^{itH} P^{ac}(H).
\end{aligned}$$

Taking into account (3.44)-(3.46), and using the completeness of W_- which yields $W_-^* = \text{s-lim}_{t\to-\infty} e^{itH_D} e^{-itH} P^{ac}(H)$, we get:

$$\begin{aligned}
&\text{s-}\lim_{t\to+\infty} U(t)\varrho_\alpha(t)U(t)^* P^{ac}(H) \\
&\qquad = \text{s-}\lim_{t\to+\infty} U(t)\Omega_-(H_D+\tau)^{-2} e^{itH_D}\widehat{\varrho}_D(H_D+\tau)^{-2} W_-^*.
\end{aligned}$$

Since $(\Omega_- - I)(H_D + \tau)^{-2}$ is also compact (its adjoint is compact, see (3.45)), we have:

$$\text{s-}\lim_{t\to+\infty} (\Omega_- - I)(H_D+\tau)^{-2} e^{itH_D} P^{ac}(H_D) = 0.$$

Thus:

$$\begin{aligned}
&\text{s-}\lim_{t\to+\infty} U(t)\varrho_\alpha(t)U(t)^*P^{ac}(H) = \\
&\quad \text{s-}\lim_{t\to+\infty} U(t)e^{itH_D}(H_D+\tau)^{-2}\widehat{\varrho}_D(H_D+\tau)^{-2}W_-^* \\
&\quad = \text{s-}\lim_{t\to+\infty} U(t)e^{itH_D}\varrho_D W_-^* = \text{s-}\lim_{t\to+\infty} U(t)e^{itH}P^{ac}(H)W_-\varrho_D W_-^*.
\end{aligned}$$

Finally, we apply (3.44) once again, and (3.43) is proved.

Now let us prove the three technical results announced in (3.44)-(3.46). We start with (3.44).

We have the identity:

$$(U(t)^* - e^{itH})(H+\tau)^{-2} = (U(t)^*(H+\tau)^{-2}e^{-itH} - (H+\tau)^{-2})e^{itH}. \tag{3.47}$$

Then by adding and subtracting several terms we can write another identity:

$$\begin{aligned}
&(U(t)^* - e^{itH})(H+\tau)^{-2} \\
&\quad = \left\{U(t)^*(H+\tau)^{-2}e^{-itH} - \widehat{\Omega}_+\right\}e^{itH} &(3.48)\\
&\quad + \left\{\widehat{\Omega}_+ - J(0)\right\}e^{itH}g + \left\{J(0) - (H+\tau)^{-2}\right\}e^{itH}. &(3.49)
\end{aligned}$$

By (3.32) we get

$$\lim_{t\to+\infty} \|U(t)^*(H+\tau)^{-2}e^{-itH} - \widehat{\Omega}_+\| = 0. \tag{3.50}$$

which shows that (3.48) tends to zero as $t \to +\infty$. Next, from (3.4), (3.26) and (3.29) we get

$$\begin{aligned}
&U(t)^*J(t)e^{-itH} - J(0) \\
&\quad = i\int_0^t ds\; e^{-\alpha s}U(s)^*(H+\tau)^{-1/2}(I+e^{-\alpha t}B)^{-1}B(H+\tau)^{-1/2}e^{-isH} \\
&\quad +\alpha\int_0^t ds\; e^{-\alpha s}U(s)^*(H+\tau)^{-1/2}(I+e^{-\alpha s}B)^{-2}B(H+\tau)^{-3/2}e^{-isH},
\end{aligned}$$

which yields

$$\begin{aligned}
&\widehat{\Omega}_+ - J(0) \\
&\quad = i\int_0^\infty ds\; e^{-\alpha s}U(s)^*(H+\tau)^{-1/2}(I+e^{-\alpha s}B)^{-1}B(H+\tau)^{-1/2}e^{-isH} \\
&\quad +\alpha\int_0^\infty ds\; e^{-\alpha s}U(s)^*(H+\tau)^{-1/2}(I+e^{-\alpha s}B)^{-2}B(H+\tau)^{-3/2}e^{-isH}.
\end{aligned}$$

Since B is a compact (rank 2) operator, we get that $\widehat{\Omega}_+ - J(0)$ is a compact operator. This fact immediately implies (via the RAGE theorem):

$$\text{s-}\lim_{t\to+\infty} (\widehat{\Omega}_+ - J(0))e^{itH}P^{ac}(H) = 0. \tag{3.51}$$

Furthermore, we have the identity:

$$\begin{aligned} &J(0) - (H+\tau)^{-2} \\ &\quad = \left((H_\alpha(0)+\tau)^{-1} - (H+\tau)^{-1}\right)(H+\tau)^{-1} \\ &\quad = -(H+\tau)^{-1/2}(I+B)^{-1}B(H+\tau)^{-3/2}, \end{aligned}$$

which gives that $J(0) - (H+\tau)^{-2}$ is compact. Thus:

$$\text{s-}\lim_{t\to+\infty}(J(0) - (H+\tau)^{-2})e^{itH}P^{ac}(H) = 0. \tag{3.52}$$

Taking into account (3.50), (3.51) and (3.52) we find

$$\text{s-}\lim_{t\to+\infty}(U(t)^* - e^{itH})(H+\tau)^{-2}P^{ac}(H) = 0$$

which proves (3.44).

Next we prove (3.45) (the estimate (3.46) is just an easy consequence of (3.45) via the RAGE theorem). Using (3.21) we have $\Omega_-(H_D+I)^{-2} = \widehat{\Omega}_-$. From (3.12), (3.15) and (3.17) we obtain:

$$\begin{aligned} &J_D(0) - U(t)^*J_D(t)e^{-itH_D} \\ &\quad = -i\int_t^0 ds\; e^{\alpha s}U(s)^*(H+\tau)^{-1/2}Q_B^\perp(e^{\alpha s}+B)^{-1}Q_B^\perp(H+\tau)^{-1/2}e^{-isH_D} \\ &\quad +\alpha\int_t^0 ds\; e^{\alpha s}U(s)^*(H+\tau)^{-1/2}(e^{\alpha s}+B)^{-2}B(H+\tau)^{-1/2}(H_D+\tau)^{-1}e^{-isH_D} \end{aligned}$$

and together with the fact that $Q_B^\perp$ is a rank 2 operator we find that $\widehat{\Omega}_- - J_D(0)$ is compact. Hence $\widehat{\Omega}_-^* - J_D(0)^*$ is compact, too.

Moreover, using (3.15) we get

$$\begin{aligned} &J_D(0) - (H_D+\tau)^{-2} = \\ &\quad ((H_\alpha(0)+\tau)^{-1} - (H_D+\tau)^{-1})(H_D+\tau)^{-1} = \\ &\quad -e^{\alpha t}(H+\tau)^{-1/2}Q_B^\perp(e^{\alpha t}+B)^{-1}Q_B^\perp(H+\tau)^{-1/2}(H_D+\tau)^{-1} \end{aligned}$$

which shows that $J_D(0) - (H_D+\tau)^{-2}$ is compact. Hence $J_D(0)^* - (H_D+\tau)^{-2}$ is compact.

Now use the identity:

$$(H_D+\tau)^{-2}(\Omega_-^* - I) = (\widehat{\Omega}_-^* - J_D(0)) + (J_D(0) - (H_D+\tau)^{-2}),$$

which proves (3.45). Finally, the relation (3.46) follows from (3.45) and the RAGE theorem. □

3.6 The main result

We are now ready to rigorously formulate and prove our main result, announced in the introduction:

Theorem 3.6 *Let H and $H_\alpha(t)$, $t \in \mathbb{R}$, $\alpha > 0$, be given by* (1.1)-(1.4) *and* (1.21)-(1.22)*, respectively. Let W_- be the incoming wave operator from* (1.26)*. Further, let $E_H(\cdot)$ and $\{\lambda_j\}_{j=1}^N$ be the spectral measure and the eigenvalues of H. If ϱ_D is a steady state for the system $\{\mathfrak{H}, H_D\}$ such that the operator $\widehat{\varrho}_D := (H_D + \tau)^4 \varrho_D$ is bounded, then the limit*

$$\varrho_\alpha := \text{s-}\lim_{T\to+\infty} \frac{1}{T} \int_0^T dt\ \varrho_\alpha(t) = \tag{3.53}$$
$$\sum_{j=1}^N E_H(\{\lambda_j\}) S_\alpha \varrho_D S_\alpha^* E_H(\{\lambda_j\}) + W_- \varrho_D W_-^*$$

exists and defines a steady state for the system $\{\mathfrak{H}, H\}$ where $S_\alpha := \Omega_+^* \Omega_-$.

Remark 3.7 We stress once again that only the part corresponding to the pure point spectrum $\varrho_\alpha^p := \sum_{j=1}^N E_H(\{\Lambda_j\}) S_\alpha \varrho_D S_\alpha^* E_H(\{\lambda_j\})$ of the steady state ϱ_α depends on the parameter $\alpha > 0$ while the absolutely continuous part $\varrho_\alpha^{ac} := W_- \varrho_D W_-^*$ does not. Note that with respect to the decomposition $\mathfrak{H} = \mathfrak{H}^p(H) \oplus \mathfrak{H}^{ac}(H)$, one has $\varrho_\alpha = \varrho_\alpha^p \oplus \varrho_\alpha^{ac}$.

Proof. By Proposition 3.5 we have

$$\text{s-}\lim_{T\to+\infty} \frac{1}{T} \int_0^T dt\ \varrho_\alpha(t) P^{ac}(H) = W_- \varrho_D W_-^*. \tag{3.54}$$

In particular, this yields:

$$\text{s-}\lim_{T\to+\infty} \frac{1}{T} \int_0^T dt\ P^s(H) \varrho_\alpha(t) P^{ac}(H) = 0,$$

where $P^s(H)$ is the projection onto the singular subspace of H. Now we are going to prove

$$\text{s-}\lim_{T\to+\infty} \frac{1}{T} \int_0^T P^{ac}(H) \varrho_\alpha(t) P^s(H) dt = 0. \tag{3.55}$$

By (3.32) we find

$$\lim_{t\to\infty} \| U(t) \Omega_- \varrho_D \Omega_-^* U(t)^* (I + H)^{-2} e^{-itH} - U(t) \Omega_- \varrho_D \Omega_-^* \widehat{\Omega}_+ \| = 0,$$

which yields

$$\lim_{t\to\infty} \| U(t) \Omega_- \varrho_D \Omega_-^* U(t)^* (I + H)^{-2} - U(t) \Omega_- \varrho_D \Omega_-^* \widehat{\Omega}_+ e^{itH} \| = 0.$$

Let λ_j be an eigenvalue of H with corresponding to an eigenfunction ϕ_j. Then

$$\lim_{t\to\infty} \|U(t)\Omega_-\varrho_D\Omega_-^* U(t)^*(I+H)^{-2}\phi_j - e^{it\lambda_j}U(t)\Omega_-\varrho_D\Omega_-^*\widehat{\Omega}_+\phi_j\| = 0.$$

This and the unitarity of Ω_+^* give:

$$\lim_{t\to\infty} \|\varrho_\alpha(t)(I+H)^{-2}\phi_j - e^{it\lambda_j}e^{-itH}\Omega_+^*\Omega_-\varrho_D\Omega_-^*\Omega_+(H+\tau)^{-2}\phi_j\| = 0$$

or

$$\lim_{t\to\infty} \|\varrho_\alpha(t)\phi_j - e^{it\lambda_j}e^{-itH}\Omega_+^*\Omega_-\varrho_D\Omega_-^*\Omega_+\phi_j\| = 0. \tag{3.56}$$

Hence we have

$$\frac{1}{T}\int_0^T dt\ P^{ac}(H)\varrho_\alpha(t)\phi_j = \frac{1}{T}\int_0^T dt\ e^{it\lambda_j}e^{-itH}P^{ac}(H)\Omega_+^*\Omega_-\varrho_D\Omega_-^*\Omega_+\phi_j.$$

We use the decomposition

$$\begin{aligned}
&\frac{1}{T}\int_0^T P^{ac}(H)\varrho_\alpha(t)\phi_j \\
&\quad= \frac{1}{T}\int_0^T dt\ e^{it\lambda_j}e^{-itH}E_H(|\lambda-\lambda_j|<\epsilon)P^{ac}(H)\Omega_+^*\Omega_-\varrho_D\Omega_-^*\Omega_+\phi_j \\
&\quad+\frac{1}{T}\int_0^T dt\ e^{it\lambda_j}e^{-itH}E_H(|\lambda-\lambda_j|\geq\epsilon)P^{ac}(H)\Omega_+^*\Omega_-\varrho_D\Omega_-^*\Omega_+\phi_j.
\end{aligned}$$

If ϵ is small enough, then $E_H(|\lambda-\lambda_j|<\epsilon)P^{ac}(H)=0$. This yields the estimate:

$$\begin{aligned}
&\left\|\frac{1}{T}\int_0^T P^{ac}(H)\varrho_\alpha(t)\phi_j\right\| \\
&\quad\leq \frac{2}{T}\left\|(H-\lambda_j)^{-1}E_H(|\lambda-\lambda_j|\geq\epsilon)P^{ac}(H)\Omega_+^*\Omega_-\varrho_D\Omega_-^*\Omega_+\phi_j\right\|
\end{aligned}$$

which immediately shows that

$$\text{s-}\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\ P^{ac}(H)\varrho_\alpha(t)\phi_j = 0, \tag{3.57}$$

and (3.55) is proved. Next, from (3.56) we easily obtain:

$$\text{s-}\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\ P^s(H)\varrho_\alpha(t)\phi_j = E_H(\{\lambda_j\})\,S_\alpha\,\varrho_D\,S_\alpha^*E_H(\{\lambda_j\}). \tag{3.58}$$

Now put together (3.54), (3.55), (3.57) and (3.58), and the proof of (3.53) is over. Now the operator ϱ_α is non-negative, bounded, and commutes with H. Hence ϱ_α is a steady state for $\{\mathfrak{H}, H\}$. □

Corollary 3.8 *Let H and $H_\alpha(t)$, $t \in \mathbb{R}$, $\alpha > 0$, be given by* (1.1)-(1.4) *and* (1.21)-(1.22)*, respectively. Then with respect to the spectral representation $\{L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu), M\}$ of H the distribution function $\{\tilde{\rho}_\alpha(\lambda)\}_{\lambda\in\mathbb{R}}$ of the steady state ϱ_α is given by*

$$\tilde{\rho}_\alpha(\lambda) := \begin{cases} 0, & \lambda \in \mathbb{R} \setminus \sigma(H) \\ \rho_{\alpha,j}, & \lambda = \lambda_j, \quad j = 1, \ldots, N \\ \mathfrak{f}_b(\lambda - \mu_b), & \lambda \in [v_b, v_a) \\ \begin{pmatrix} \mathfrak{f}_b(\lambda - \mu_b) & 0 \\ 0 & \mathfrak{f}_a(\lambda - \mu_a) \end{pmatrix}, & \lambda \in [v_a, \infty) \end{cases} \tag{3.59}$$

where $\rho_{\alpha,j} := (S_\alpha \phi_j, \phi_j)$, $j = 1, 2, \ldots, N$.

Proof. Using the generalized Fourier transform (2.2)-(2.4) one has to consider the operator $\Phi^{-1}\varrho_a\Phi : L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu) \longrightarrow L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$. Using the representations

$$\Phi\varrho_\alpha\Phi^{-1} = \Phi\varrho_\alpha^p\Phi^{-1} + \Phi\varrho_\alpha^{ac}\Phi^{-1}$$

and

$$\Phi\varrho_\alpha^{ac}\Phi^{-1} = \Phi W_-\varrho_D^{ac}W_-^*\Phi^{-1} = \Phi W_-\Psi^{-1}\Psi\varrho_D^{ac}\Psi^{-1}\Psi W_-^*\Phi^{-1},$$

$\varrho_D^{ac} := \varrho_a \oplus \varrho_b$, we get

$$M(\tilde{\rho}_\alpha^{ac}) = \Phi W_-\Psi^{-1}M(\tilde{\rho}_D^{ac})\Psi W_-^*\Phi^{-1}.$$

where

$$\tilde{\rho}_D^{ac}(\lambda) := \begin{cases} 0, & \lambda \in \mathbb{R} \setminus \sigma_{ac}(H) \\ \mathfrak{f}_b(\lambda - \mu_b) & \lambda \in [v_b, v_a) \\ \begin{pmatrix} \mathfrak{f}_b(\lambda - \mu_b) & 0 \\ 0 & \mathfrak{f}_a(\lambda - \mu_a \end{pmatrix}, & \lambda \in [v_a, \infty). \end{cases} \tag{3.60}$$

Taking into account (2.5) we prove (3.59). □

3.7 The case of sudden coupling

Let us compare our results with following model [4]. Assume that our system is not coupled for $t < 0$ and suddenly at $t = 0$ the system becomes fully coupled. In a more mathematical manner this can be modeled by the following family of self-adjoint operators:

$$\widetilde{H}(t) := \begin{cases} H_D & t < 0 \\ H & t \geq 0. \end{cases}$$

To the evolution equation

$$i\frac{\partial}{\partial t}u(t) = \widetilde{H}(t)u(t), \quad t \in \mathbb{R},$$

it corresponds a unique unitary solution operator or propagator $\{\widetilde{U}(t,s)\}_{(t,s)\in\mathbb{R}\times\mathbb{R}}$ given by

$$\widetilde{U}(t,s) := \widetilde{U}(t)\widetilde{U}(s)^{-1}, \quad t,s\in\mathbb{R},$$

where

$$\widetilde{U}(t) = \begin{cases} e^{-itH_D}, & t\leq 0 \\ e^{-itH}, & t>0. \end{cases}$$

The time evolution of the density operator is given by

$$\varrho_\infty(t) := \widetilde{U}(t)\varrho_D\widetilde{U}(t)^*, \quad t>0.$$

Clearly, $\lim_{t\to-\infty}\|\varrho_\infty(t)-\varrho_D\|=0$. Then using the identity:

$$\widetilde{\varrho}(t) = e^{-itH}e^{itH_D}\varrho_D e^{-itH_D}e^{itH}, \quad t>0,$$

we immediately get that

$$\text{s-}\lim_{t\to+\infty}\varrho_\infty(t)P^{ac}(H) = W_-\varrho_D W_-^*.$$

Hence we find

$$\text{s-}\lim_{T\to+\infty}\frac{1}{T}\int_0^T dt\ \varrho_\infty(t)P^{ac}(H) = W_-\varrho_D W_-^*.$$

As above, we can show that

$$\text{s-}\lim_{T\to+\infty}\frac{1}{T}\int_0^T dt\ P^{ac}(H)\varrho_\infty(t)P^{s}(H) = 0$$

and

$$\text{s-}\lim_{T\to+\infty}\frac{1}{T}\int_0^T dt\ P^{s}(H)\varrho_\infty(t)P^{s}(H) = \sum_{j=1}^N E_H(\{\lambda_j\})\varrho_D E_H(\{\lambda_j\}).$$

Hence we find

$$\text{s-}\lim_{T\to+\infty}\frac{1}{T}\int_0^T dt\ \varrho_\infty(t) = \sum_{j=1}^N E_H(\{\lambda_j\})\varrho_D E_H(\{\lambda_j\}) + W_-\varrho_D W_-^*.$$

4 The stationary current, the Landau-Lifschitz and the Landauer-Büttiker formula

There are by now several proofs of the Landauer-Büttiker formula in the NESS approach (see [4, 26]), and in the finite volume regularization approach (see [12, 13, 14]). Here we give yet another proof in the NESS approach. In fact, we will only justify the so-called Landau-Lifschitz current density formula (see (4.4) in what follows), which was the starting point in [6] for the proof of the Landauer-Büttiker formula (see Example 5.11 in that paper).

Let us start by defining the stationary current, in the manner introduced in [4]. Let $\eta > 0$, and choose an integer $N \geq 2$. Denote by χ_b the characteristic function of the interval (b, ∞) (the right reservoir). Without loss of generality, let us assume that $H > 0$.

Definition 4.1 *The trace class operator*

$$j(\eta) := i[H(1+\eta H)^{-N}, \chi_b]$$

is called the regularized current operator. The stationary current coming out of the right reservoir is defined to be

$$\mathfrak{I}_\alpha := \lim_{\eta \searrow 0} \mathrm{Tr}(\varrho_\alpha j(\eta)).$$

Now a few comments. The current operator is trace class because we can write it as

$$i[H(1+\eta H)^{-N} - H_D(1+\eta H_D)^{-N}, \chi_b]$$

which clearly is trace class. Since ϱ_α^p does not contribute to the trace in the definition of the current, we will focus on the clearly α independent quantity:

$$\mathfrak{I} = \lim_{\eta \searrow 0} \mathrm{Tr}\left\{W_- \varrho_D W_-^* P^{ac}(H) j(\eta)\right\}.$$

We start with a technical result:

Lemma 4.2 *Let χ a bounded, compactly supported function. Then the operator $\chi(1+H)^{-2}$ is trace class.*

Proof. Choose a smooth and compactly supported function $\tilde{\chi}$ such that $\tilde{\chi}\chi = \chi$. Write

$$\chi(1+H)^{-2} = \chi\tilde{\chi}(1+H)^{-2} = \chi(1+H)^{-1}\tilde{\chi}(1+H)^{-1} + \chi(1+H)^{-2}[H,\tilde{\chi}](1+H)^{-1}.$$

Since $\tilde{\chi}$ is smooth and compactly supported, the operator $(1+H)^{-1}[H,\tilde{\chi}](1+H)^{-1}$ is Hilbert-Schmidt. The operators $\chi(1+H)^{-1}$ and $\tilde{\chi}(1+H)^{-1}$ are also Hilbert-Schmidt, thus $\chi(1+H)^{-2}$ can be written as a sum of products of Hilbert-Schmidt operators, therefore it is trace class. □

Next, let us now prove that we can replace the sharp characteristic function in the definition of the current by a smooth one. Let $c > b+1$. Choose any function $\phi_c \in C^\infty(\mathbb{R})$ such that

$$0 \leq \phi_c \leq 1, \quad \phi_c(x) = 1 \text{ if } x \geq c+1, \quad \mathrm{supp}(\phi_c) \subset (c-1, \infty). \tag{4.1}$$

Then let us prove the following identity:

Lemma 4.3 *Let $c > b+1$ and let $\phi_c \in C^\infty(\mathbb{R})$ such that the conditions* (4.1) *are satisfied. If ϱ_D is a steady state for the system $\{\mathfrak{H}, H_D\}$ such that the operator $\widehat{\varrho}_D := (H_D+\tau)^4\varrho_D$ is bounded, then*

$$\begin{aligned} &\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H) j(\eta)\right\} = \\ &\quad i\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H)[H(1+\eta H)^{-N}, \phi_c]\right\}. \end{aligned} \tag{4.2}$$

Proof. First, the commutator $[H(1+\eta H)^{-N}, \phi_c]$ defines a trace class operator; that is because now $[H,\phi_c] = -\frac{1}{2m_b}(\frac{d}{dx}\phi_c' + \phi_c'\frac{d}{dx})$, and $(1+\eta H)^{-1}[H,\phi_c](1+\eta H)^{-1}$ is a trace class operator (we can write it as a sum of products of two Hilbert-Schmidt operators). We also use the identity

$$W_-\varrho_D W_-^* P^{ac}(H) = W_-\varrho_D(1+H_D)W_-^* P^{ac}(H)(1+H)^{-1}$$

which is an easy consequence of the intertwining property of W_-.

Second, (4.2) would be implied by:

$$\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H)[H(1+\eta H)^{-N}, \phi_c - \chi_b]\right\} = 0.$$

We see that $\phi_c - \chi_b$ has compact support. If we write the commutator as the difference of two terms, both of them will be trace class. The first one is

$$\begin{aligned} &W_-\varrho_D W_-^* P^{ac}(H) H(1+\eta H)^{-N}(\phi_c - \chi_b) \\ &= W_-\varrho_D(1+H_D)^2 W_-^* P^{ac}(H) H(1+\eta H)^{-N}\{(1+H)^{-2}(\phi_c-\chi_b)\} \end{aligned}$$

and the second one is

$$\begin{aligned} &W_-\varrho_D W_-^* P^{ac}(H)(\phi_c - \chi_b) H(1+\eta H)^{-N} \\ &= W_-\varrho_D(1+H_D)^2 W_-^* P^{ac}(H)\{(1+H)^{-2}(\phi_c-\chi_b)\} H(1+\eta H)^{-N}. \end{aligned}$$

Now according to Lemma 4.2, $(1+H)^{-2}(\phi_c-\chi_b)$ is a trace class operator. Thus the two traces will be equal due to the cyclicity property and the fact that H commutes with the steady state. □

We can now take the limit $\eta \searrow 0$:

Lemma 4.4 *The operator $(1+H)^{-2}[H,\phi_c]$ is trace class, and*

$$\mathfrak{I} = i\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H)[H,\phi_c]\right\}, \tag{4.3}$$

independent of ϕ_c.

Proof. Note that $[H,\phi_c] = -\frac{1}{2m_b}(2\frac{d}{dx}\phi_c' - \phi_c'')$, where both ϕ_c' and ϕ_c'' are compactly supported. Using the method of Lemma 4.2 one can prove that $(1+H)^{-2}\frac{d}{dx}\phi_c'$ is trace class, hence $(1+H)^{-2}[H,\phi_c]$ is trace class. Thus $W_-\varrho_D W_-^* P^{ac}(H)[H,\phi_c]$ is trace class since we can write

$$W_-\varrho_D W_-^* P^{ac}(H)[H,\phi_c] = W_-\varrho_D(1+H_D)^2 W_-^* P^{ac}(H)(1+H)^{-2}[H,\phi_c].$$

In fact, using trace cyclicity one can prove that

$$\begin{aligned}&\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H)[H,\phi_c]\right\} = \\ &\quad \mathrm{Tr}\left\{W_-\varrho_D(1+H_D)^2 W_-^* P^{ac}(H)(1+H)^{-1}[H,\phi_c](1+H)^{-1}\right\} \\ &\quad = -\mathrm{Tr}\left\{W_-\varrho_D(1+H_D)^2 W_-^* P^{ac}(H)[(1+H)^{-1},\phi_c]\right\}.\end{aligned}$$

This last identity indicates the strategy of the proof. Write:

$$\begin{aligned}&\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H)[H(1+\eta H)^{-N},\phi_c]\right\} \\ &= \mathrm{Tr}\left\{W_-\varrho_D(1+H_D)^3 W_-^* P^{ac}(H)(1+H)^{-2}[H(1+\eta H)^{-N},\phi_c](1+H)^{-1}\right\}.\end{aligned}$$

Now it is not so complicated to prove that $(1+H)^{-2}[H(1+\eta H)^{-N},\phi_c](1+H)^{-1}$ converges in the trace norm to $(1+H)^{-2}[H,\phi_c](1+H)^{-1}$ when $\eta \searrow 0$; we do not give details. Now use (4.2) and take the limit; we obtain:

$$\begin{aligned}\mathfrak{I} &= i\mathrm{Tr}\left\{W_-\varrho_D(1+H_D)^3 W_-^* P^{ac}(H)(1+H)^{-2}[H,\phi_c](1+H)^{-1}\right\} \\ &= i\mathrm{Tr}\left\{W_-\varrho_D W_-^* P^{ac}(H)[H,\phi_c]\right\},\end{aligned}$$

where in the last line we used trace cyclicity. □

We are going to compute the trace in (4.3) using the spectral representation of H. Let us compute the integral kernel of $\mathcal{A} := iW_-\varrho_D W_-^* P^{ac}(H)\frac{1}{2m_b}\left(-\frac{d}{dx}\phi_c' - \phi_c'\frac{d}{dx}\right)$ in this representation. We use (3.60), where we denote the diagonal elements of $\tilde{\varrho}_D^{ac}(\lambda)$ by $\tilde{\varrho}_D^{ac}(\lambda)_{pp}$ (the other entries are zero). We obtain:

$$\begin{aligned}&\mathcal{A}(\lambda,p;\lambda',p') = \\ &\quad -\frac{i}{2m_b}\tilde{\varrho}_D^{ac}(\lambda)_{pp}\int_{\mathbb{R}}\overline{\tilde{\phi}_p(x,\lambda)}\left(\frac{d}{dx}\phi_c'(x)+\phi_c'(x)\frac{d}{dx}\right)\tilde{\phi}_{p'}(x,\lambda')dx \\ &\quad = -\frac{i}{2m_b}\tilde{\varrho}_D^{ac}(\lambda)_{pp}\int_{\mathbb{R}}\phi_c'(x)\{\overline{\tilde{\phi}_p(x,\lambda)}\tilde{\phi}_{p'}'(x,\lambda') - \overline{\tilde{\phi}_p'(x,\lambda)}\tilde{\phi}_{p'}(x,\lambda')\}dx,\end{aligned}$$

where in the second line we integrated by parts (remember that ϕ_c' is compactly supported).

In order to compute the trace, we put $\lambda = \lambda'$, $p = p'$, and integrate/sum over the variables. We obtain:

$$\mathfrak{I} = \int_{\mathbb{R}}\phi_c'(x)j(x)dx,$$

where

$$j(x) := \frac{1}{m_b}\int_{v_b}^{\infty}\sum_p \tilde{\varrho}_D^{ac}(\lambda)_{pp}\mathrm{Im}\,\{\overline{\tilde{\phi}_p(x,\lambda)}\tilde{\phi}_p'(x,\lambda)\}d\lambda \tag{4.4}$$

is the current density, which is independent of x (the above imaginary part is a Wronskian of two solutions of a Schrödinger equation, see [6] for details). But $\int_{\mathbb{R}}\phi_c'(x)dx = 1$ for our class of cut-off functions, therefore the stationary current

equals the (constant) value of its density. The Landauer-Büttiker formula follows from the Landau-Lifschitz formula (4.4) as proved in [6].

Acknowledgments H.C. and H.N. acknowledge support from the Danish F.N.U. grant *Mathematical Physics and Partial Differential Equations*. This work was initiated during a visit of H.C. and V.Z. at WIAS, and they are thankful for the hospitality and financial support extended to them during the work on this paper.

References

[1] T. Aktosun. On the Schrödinger equation with steplike potentials. *J. Math. Phys.*, 40(11):5289–5305, 1999.

[2] T. Aktosun. Darboux transformation for the Schrödinger equation with steplike potentials. *J. Math. Phys.*, 41(4):1619–1631, 2000.

[3] W. O. Amrein and Ph. Jacquet. Time delay for one-dimensional quantum systems with steplike potentials. Preprint, arXiv:quant-ph/0610198, 2006.

[4] W. Aschbacher, V. Jakšić, Y. Pautrat, and C.-A. Pillet. Transport properties of quasi-free fermions. *J. Math. Phys.*, 48(3):032101, 28, 2007.

[5] M. Baro, N. Ben Abdallah, P. Degond, and A. El Ayyadi. A 1D coupled Schrödinger drift-diffusion model including collisions. *J. Comput. Phys.*, 203(1):129–153, 2005.

[6] M. Baro, H.-Chr. Kaiser, H. Neidhardt, and J. Rehberg. A quantum transmitting Schrödinger-Poisson system. *Rev. Math. Phys.*, 16(3):281–330, 2004.

[7] M. Baro, H. Neidhardt, and J. Rehberg. Current coupling of drift-diffusion models and Schrödinger-Poisson systems: dissipative hybrid models. *SIAM J. Math. Anal.*, 37(3):941–981, 2005.

[8] V. Buslaev and V. Fomin. An inverse scattering problem for the one-dimensional Schrödinger equation on the entire axis. *Vestnik Leningrad. Univ.*, 17(1):56–64, 1962.

[9] M. Cini. Time-dependent approach to electron transport through junctions: General theory and simple applications. *Phys. Rev. B.*, 22, 1980.

[10] A. Cohen. A counterexample in the inverse scattering theory for steplike potentials. *Comm. Partial Differential Equations*, 7(8):883–904, 1982.

[11] A. Cohen and Th. Kappeler. Scattering and inverse scattering for steplike potentials in the Schrödinger equation. *Indiana Univ. Math. J.*, 34(1):127–180, 1985.

[12] H. D. Cornean, P. Duclos, G. Nenciu, and R. Purice. Adiabatically switched-on electrical bias in continuous systems, and the Landauer-Büttiker formula. Preprint, arXiv:0708.0303, 2007.

[13] H. D. Cornean, A. Jensen, and V. Moldoveanu. A rigorous proof of the Landauer-Büttiker formula. *J. Math. Phys.*, 46(4):042106, 28, 2005.

[14] H. D. Cornean, A. Jensen, and V. Moldoveanu. The Landauer-Büttiker formula and resonant quantum transport. In *Mathematical physics of quantum mechanics*, volume 690 of *Lecture Notes in Phys.*, pages 45–53. Springer, Berlin, 2006.

[15] W. R. Frensley. Quantum transport. In Norman G. Einspruch and William R. Frensley, editors, *Heterostructures and quantum devices*.

[16] W. R. Frensley. Boundary conditions for open quantum systems driven far from equilibrium. *Rev. Modern Phys.*, 62:745–791, 1990.

[17] H. Gajewski. Analysis und Numerik von Ladungstransport in Halbleitern. *Mitt. Ges. Angew. Math. Mech.*, 16(1):35–57, 1993.

[18] F. Gesztesy, R. Nowell, and W. Pötz. One-dimensional scattering theory for quantum systems with nontrivial spatial asymptotics. *Differential Integral Equations*, 10(3):521–546, 1997.

[19] V. Jakšić and C.-A. Pillet. Mathematical theory of non-equilibrium quantum statistical mechanics. *J. Statist. Phys.*, 108(5-6):787–829, 2002.

[20] D. Kirkner and C. Lent. The quantum transmitting boundary method. *J. Appl. Phys.*, 67:6353–6359, 1990.

[21] J. Kisyński. Sur les opérateurs de Green des problèmes de Cauchy abstraits. *Studia Math.*, 23:285–328, 1963/1964.

[22] P. A. Markowich. *The stationary semiconductor device equations*. Computational Microelectronics. Springer-Verlag, Vienna, 1986.

[23] V. Moldoveanu, V. Gudmundsson, and A. Manolescu. Transient regime in nonlinear transport through many-level quantum dots. *Phys. Rev. B.*, 76:085330, 2007.

[24] C. M. Naón, M. J. Salvay, and M. L. Trobo. Effect of nonadiabatic switching of dynamic perturbations in one-dimensional fermi systems. *Phys. Rev. B.*, 70:195109.

[25] H. Neidhardt and V. A. Zagrebnov. Linear non-autonomous cauchy problems and evolution semigroups. Preprint, arXiv:0711:0284, 2007.

[26] G. Nenciu. Independent electron model for open quantum systems: Landauer-Büttiker formula and strict positivity of the entropy production. *J. Math. Phys.*, 48(3):033302, 8, 2007.

[27] F. Nier. The dynamics of some quantum open systems with short-range nonlinearities. *Nonlinearity*, 11(4):1127–1172, 1998.

[28] W. Pötz. Scattering theory for mesoscopic quantum systems with non-trivial spatial asymptotics in one dimension. *J. Math. Phys.*, 36(4):1707–1740, 1995.

[29] S. Selberherr. *Analysis and Simulation of Semiconductor Devices*. Springer Verlag, Wien, 1984.

[30] G. Stefanucci. Bound states in *ab initio* approaches to quantum transport: A time-dependent formulation. *Phys. Rev. B.*, 75:195115, 2007.

[31] G. Stefanucci and C.-O. Almbladh. Time-dependent partition-free approach in resonant tunneling systems. *Phys. Rev. B.*, 69:195318, 2004.

[32] B. Vinter and C. Weisbuch. *Quantum Semiconductor Structures: Fundamentals and Applications*. Academic Press, Boston, 1991.

[33] D. R. Yafaev. *Mathematical scattering theory*, volume 105 of *Translations of Mathematical Monographs*. American Mathematical Society, Providence, RI, 1992.