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Density and current of a dissipative Schrödinger operator

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Abstract

A net current flow through an open 1-dimensional Schrödinger-Poisson system is modeled by replacing self-adjoint boundary conditions by dissipative ones. To give a rigorous definition of carrier and current densities the well-known dilation theory of dissipative operators is used where the self-adjoint dilation is regarded as the Hamiltonian of a larger closed system which contains the open one. The carrier density turns out to be performed by the generalized eigenstates of the dilation while the current density is related to the characteristic function of the dissipative operator. A rigorous setup of a dissipative Schrödinger-Poisson system is outlined.

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Keywords

open Schrödinger-Poisson system, carrier and current density, dissipative Schrödinger operator, self-adjoint dilation, generalized eigenfunctions, characteristic function, density matrix

Contents

1 Introduction

Schrödinger-Poisson systems are of great interest in semiconductor physics. In the following we are interested in a Schrödinger-Poisson system on the interval $\Omega = [a, b]$ on the real axis $\mathbb{R}$. Systems of this type were considered in [9]. By φ we denote the electrostatic potential on Ω which is determined by Poisson's equation

$$-\frac{d}{dx}\epsilon(x)\frac{d}{dx}\varphi = q\left(C(x) + u^+ - u^-\right), \quad x \in \Omega, \tag{1.1}$$

where u^+ and u^- are the densities of holes and electrons, q is the magnitude of the elementary charge, $C(\cdot)$ is the so-called doping profile of the semiconductor devices and $\epsilon = \epsilon(x) > 0$ denotes the dielectric permittivity which satisfies the condition

$$\epsilon(\cdot) + \frac{1}{\epsilon(\cdot)} \in L^\infty([a, b]). \tag{1.2}$$

The Poisson equation (1.1) is completed by the boundary conditions

$$\varphi(a) = \varphi_a, \quad \text{and} \quad \varphi(b) = \varphi_b. \tag{1.3}$$

The second important ingredient of the Schrödinger-Poisson system are Schrödinger-type operators H which are defined on the Hilbert space $\mathfrak{H} = L^2([a, b])$ and look like

$$H := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx} + V, \tag{1.4}$$

where the real potential V is slightly different for holes and electrons, see Section 5, and m equals either to the x-dependent effective mass of the holes or of the electrons. Since the formalism of quantum mechanics is well developed only for self-adjoint operators usually self-adjoint boundary conditions, for instance Neuman or Dirichlet boundary conditions at a and b, are chosen. Operators of this type have a discrete spectrum. Let us denote by $\{\mathcal{E}_l\}_{l=1}^\infty$ and $\{\psi_l\}_{l=1}^\infty$ the sequence of eigenvalues and eigenfunctions counting multiplicities.

The carrier densities used in the Poisson equation are now performed by expressions of the form

$$u_{\hat{\varrho}}(x) = \sum_{l=1}^\infty \varrho_l |\psi_l(x)|^2, \quad x \in [a, b], \tag{1.5}$$

where $\hat{\varrho} := \{\varrho_l\}_{l=1}^\infty$ is a sequence of occupation numbers such that

$$N := \sum_{l=1}^\infty \varrho_l, \tag{1.6}$$

is the total number of carriers of the system. Usually, the sequence $\hat{\varrho}$ is given by

$$\varrho_l := f(\mathcal{E}_l), \quad l = 1, 2, \ldots. \tag{1.7}$$

where $f \geq 0$ is a equilibrium distribution functions which may be different for holes and electrons. Let us introduce the operator

$$\varrho := f(H). \tag{1.8}$$

The operator ϱ is self-adjoint and non-negative. If the equilibrium distribution function f tends to zero sufficiently fast as $x \to +\infty$, then ϱ is nuclear. From ϱ one computes the total number N of carriers by $N = \mathrm{tr}(\varrho) = \mathrm{tr}(f(H))$. Usually, non-negative self-adjoint nuclear operators are called density matrices. Since ϱ commutes with H the density matrix ϱ remains unchanged in time. In this case ϱ is called a steady state. If the density matrix is known, then one restores the carrier density as follows: the number of carriers $N_\varrho(\omega)$ in the set $\omega \subseteq [a, b]$ is computed by

$$N_\varrho(\omega) = \mathrm{tr}(\varrho\chi_\omega), \tag{1.9}$$

where $\chi_\omega(\cdot)$ is the indicator function of the subset ω. It turns out that (1.9) defines an absolutely continuous measure (with respect to the Lebesgue measure). One verifies that its Radon-Nikodym derivative u_ϱ coincides with the carrier density defined by (1.5), i.e. $u_{\hat{\varrho}} = u_\varrho$.

The system described by H is closed. Hence there is no interaction with the environment, in particular, no carrier exchange. Consequently, the current density $j_{\hat{\varrho}}(x)$ defined by

$$j_{\hat{\varrho}}(x) := \sum_{l=1}^{\infty} \varrho_l j_l(x), \quad x \in [a, b], \tag{1.10}$$

is identical zero, where in accordance with [15] the current density $j_l(x)$ of the eigenstate ψ_l is given by

$$j_l(x) := \Im\mathrm{m}\left(\frac{1}{m(x)}\psi_l'(x)\overline{\psi_l(x)}\right), \; x \in [a, b], \; l = 1, 2, \ldots. \tag{1.11}$$

However, from the point of view of semiconductor physics this consequence is totally unacceptable since a net current flow through the boundary is natural. Thus one has to devise boundary conditions which allow those flows.

A simple proposal was made in [9] which adds up to replace the self-adjoint boundary conditions by non-selfadjoint ones, i.e. to consider H on the domain

$$\mathrm{dom}(H) = \left\{ g \in W^{1,2}([a, b]) : \begin{array}{c} \frac{1}{m(x)}g'(x) \in W^{1,2}([a, b]), \\ \frac{1}{2m(a)}g'(a) = -\kappa_a g(a), \\ \frac{1}{2m(b)}g'(b) = \kappa_b g(b) \end{array} \right\} \tag{1.12}$$

where $\kappa_a, \kappa_b \in \mathbb{C}$. If at least one of the imaginary parts is different from zero, then the operator H is non-selfadjoint. However, this non-selfadjointness implies several complications. In particular, the notion of carrier densities becomes unclear.

This situation can be handled if we restrict ourselves to dissipative operators. Let us recall that an operator is called dissipative if the imaginary part of its associated quadratic form is non-positive. In the present case the operator H is dissipative if $\kappa_a, \kappa_b \in \mathbb{C}_+ := \{z \in \mathbb{C} : \Im\mathrm{m}(z) > 0\}$, see [11]. Moreover, under this assumption the operator H becomes maximal dissipative, i.e. it admits no proper dissipative extension, see [11]. The main technical tool to overcome the difficulties is the dilation theory for maximal dissipative operator. In [12] the minimal self-adjoint dilation K of H was explicitly constructed and analysed in detail. From the physical point of view the minimal self-adjoint dilation plays the role of the Hamiltonian of a larger closed system which contains the original system described by H. Using this fact one defines steady states, carrier densities and current densities. It turns out that the current density is independent of $x \in [a,b]$ and, in general, different from zero. So we have a constant current through $[a,b]$ which is quite satisfactory from the physical point of view.

It turns out that this formal approach to the net current flow problem fits into models discussed in the literature. Indeed, a well adopted model in semiconductor physics is the so-called Kirkner-Lent model [14] which was mathematically analysed in [4], [5] and [6]. In this model one replaces the maximal dissipative operator H by a family of maximal dissipative operators $\{H(z)\}_{z\in\overline{\mathbb{C}_+}}$ defined on $\mathfrak{H} = L^2([a,b])$ and given by

$$\begin{aligned} \mathrm{dom}(H(z)) &:= \left\{ g \in W^{2,2}([0,1]) : \begin{array}{l} g'(1) = \kappa_1(z)g(1) \\ g'(0) = -\kappa_0(z)g(0), \end{array} \right\}, \\ (H(z)g)(x) &:= -\tfrac{d^2}{dx^2}g(x) + V(x)g(x), \quad g \in \mathrm{dom}(H(z)), \end{aligned} \tag{1.13}$$

$m(x) \equiv 1/2$, with

$$\kappa_1(z) := i\sqrt{z} \quad \text{and} \quad \kappa_0(z) := i\sqrt{z - V_-}, \quad z \in \overline{\mathbb{C}_+}, \tag{1.14}$$

where the cut of the square root is along $[0,\infty)$ and $\Im\mathrm{m}(\sqrt{z}) \geq 0$ for $z \in \mathbb{C}_+$. Let us consider the self-adjoint Schrödinger operator K,

$$\begin{aligned} \mathrm{dom}(K) &:= W^{2,2}(\mathbb{R}), \\ (Kf)(x) &:= -\tfrac{d^2}{dx^2}f(x) + V_{KL}(x)f(x), \quad f \in \mathrm{dom}(K), \end{aligned} \tag{1.15}$$

on the Hilbert space $\mathfrak{K} = L^2(\mathbb{R})$ whose potential $V_{KL} \in C(\mathbb{R})$ looks like

$$V_{KL} = \begin{cases} V_- & : \; x \in \mathbb{R}_- \\ V & : \; x \in [0,1] \\ 0 & : \; x \in (1,+\infty) \end{cases} \tag{1.16}$$

where $V_- > 0$,

$$V(0) = V_- \quad \text{and} \quad V(1) = 0. \tag{1.17}$$

Operators of this type were investigate in [7]. It turns out that

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K - z)^{-1}|\mathfrak{H} = (H(z) - z)^{-1}, \quad z \in \mathbb{C}_+. \tag{1.18}$$

which means that the operator K can be regarded as a self-adjoint dilation of the family $\{H(z)\}_{z\in\overline{\mathbb{C}_+}}$. Moreover, it holds

$$\bigvee_{z\in\mathbb{C}\setminus\mathbb{R}} (K-z)^{-1}\mathfrak{H} = \mathfrak{K} \tag{1.19}$$

which means that K is a minimal self-adjoint dilation and, hence, that K is unique up to a certain isomorphism. Thus, if we want to compute quantities which are related to the subspace $\mathfrak{H}$, for instance, carrier densities on the interval $[0,1]$, we can do this using either the self-adjoint operator K or the family $\{H(\lambda)\}_{\lambda\in\mathbb{R}}$ of maximal dissipative operators. Moreover, if we are only interested in quantities with respect to a small energy interval around the energy $\lambda_0 \in \mathbb{R}$ (in the limit only quantities for the energy λ_0), then it is enough to consider the maximal dissipative operator $H(\lambda_0)$ which leads to a model described at the beginning.

The paper is organized as follows. In Section 2 we rigorously define Schrödinger-type operators and briefly recall their properties, cf. [11]. Moreover, we introduce the important notion of the characteristic function $\Theta_H(z)$ and briefly describe the minimal self-adjoint dilation K of H. For further purposes we indicate its generalized eigenfunction expansion. Essentially, we follow here the paper [12]. In Section 3 we introduce generalized steady states and define carrier densities. In Section 4 we define the current density and compute it in terms of the characteristic function. In particular, it turns out that if the steady state is given by $\varrho = f(K)$, then the current density is zero. In Section 5 we comment the results, in particular, we clarify the relation to the Lax-Phillips scattering theory and verify the continuity equation. Finally, we give a rigorous setting of so-called dissipative Schrödinger-Poisson systems which have the advantage that their current densities are different from zero for suitable chosen steady states.

2 Schrödinger-type operators

Following the proposal of [9] we consider the non-selfadjoint Schrödinger-type operator H on the Hilbert space $\mathfrak{H} = L^2([a,b])$ given by the domain (1.12) and

$$(Hg)(x) = (l(g))(x), \quad g \in \mathrm{dom}(H), \tag{2.1}$$

where

$$(l(g))(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}g(x) + V(x)g(x), \tag{2.2}$$

and $V \in L^2([a,b])$ is a real potential, the effective mass $m(x) > 0$ obeys $m(x)+\frac{1}{m(x)} \in L^\infty([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. The operator H is maximal dissipative and completely non-selfadjoint, see [11]. The spectrum of H consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity. Since the operator H is completely non-selfadjoint there do not exist real eigenvalues. To analyze the operator H it is useful to introduce the elementary solutions $v_a(x,z)$ and $v_b(x,z)$,

$$l(v_a(x,z)) - zv_a(x,z) = 0, \quad v_a(a,z) = 1, \quad \frac{1}{2m(a)}v_a'(a,z) = -\kappa_a, \tag{2.3}$$

$$l(v_b(x,z)) - zv_b(x,z) = 0, \quad v_b(b,z) = 1, \quad \frac{1}{2m(b)}v_b'(b,z) = \kappa_b, \tag{2.4}$$

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

$$W(z) = v_a(x,z)\frac{1}{2m(x)}v_b'(x,z) - v_b(x,z)\frac{1}{2m(x)}v_a'(x,z). \tag{2.5}$$

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

$$v_{*a}(x,z) := \overline{v_a(x,\overline{z})} \quad \text{and} \quad v_{*b}(x,z) := \overline{v_b(x,\overline{z})}, \quad z \in \mathbb{C}, \tag{2.6}$$

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

$$l(v_{*a}(x,z)) - zv_{*a}(x,z) = 0, \quad v_{*a}(a,z) = 1, \quad \frac{1}{2m(a)}v_{*a}'(a,z) = -\overline{\kappa_a}, \tag{2.7}$$

$$l(v_{*b}(x,z)) - zv_{*b}(x,z) = 0, \quad v_{*b}(b,z) = 1, \quad \frac{1}{2m(b)}v_{*b}'(b,z) = \overline{\kappa_b}, \tag{2.8}$$

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

$$\begin{aligned} &((H-z)^{-1}f)(x) = \\ &\qquad -\frac{v_b(x,z)}{W(z)}\int_a^x dy\, v_a(y,z)f(y) - \frac{v_a(x,z)}{W(z)}\int_x^b dy\, v_b(y,z)f(y), \end{aligned} \tag{2.9}$$

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

$$\begin{aligned} &((H^*-z)^{-1}f)(x) = \\ &\qquad -\frac{v_{*b}(x,z)}{W_*(z)}\int_a^x dy\, v_{*a}(y,z)f(y) - \frac{v_{*a}(x,z)}{W_*(z)}\int_x^b dy\, v_{*b}(y,z)f(y), \end{aligned} \tag{2.10}$$

for $z \in \varrho(H^*)$ and $f \in L^2([a,b])$, see [12].

Since H is completely non-selfadjoint the maximal dissipative operator H can be completely characterized by its characteristic function $\Theta_H(z)$, $z \in \varrho(H) \cap \varrho(H^*)$, cf. [8]. The definition of the characteristic function relies on the so-called boundary operators $T(z) : \mathfrak{H} \longrightarrow \mathbb{C}^2$, $z \in \varrho(H)$ and $T_*(z) : \mathfrak{H} \longrightarrow \mathbb{C}^2$, $z \in \varrho(H^*)$, which are defined in [12]. Writing

$$\kappa_a = q_a + \frac{i}{2}\alpha_a^2 \quad \text{and} \quad \kappa_b = q_b + \frac{i}{2}\alpha_b^2, \quad \alpha_a, \alpha_b > 0, \tag{2.11}$$

the boundary operators are defined by

$$T(z)f := \begin{pmatrix} \alpha_b((H-z)^{-1}f)(b) \\ -\alpha_a((H-z)^{-1}f)(a) \end{pmatrix} \tag{2.12}$$

and

$$T_*(z)f := \begin{pmatrix} \alpha_b((H^*-z)^{-1}f)(b) \\ -\alpha_a((H^*-z)^{-1}f)(a) \end{pmatrix}, \tag{2.13}$$

$f \in L^2([a,b])$. Using the resolvent representations (2.9) and (2.10) we obtain

$$T(z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\ v_a(y,z)f(y) \\ \alpha_a \int_a^b dy\ v_b(y,z)f(y) \end{pmatrix} \tag{2.14}$$

and

$$T_*(z)f = \frac{1}{W_*(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\ v_{*a}(y,z)f(y) \\ \alpha_b \int_a^b dy\ v_{*b}(y,z)f(y) \end{pmatrix}, \tag{2.15}$$

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

$$\begin{aligned} \left(T(z)^*\xi\right)(x) &= \frac{1}{\overline{W(z)}} \left(-\alpha_b\overline{v_a(x,z)}, \alpha_a\overline{v_b(x,z)}\right)\xi \\ &= \frac{1}{W_*(\overline{z})} \left(-\alpha_b v_{*a}(x,\overline{z}), \alpha_a v_{*b}(x,\overline{z})\right)\xi, \end{aligned} \tag{2.16}$$

and

$$\begin{aligned} \left(T_*(z)^*\xi\right)(x) &= \frac{1}{\overline{W_*(z)}} \left(-\alpha_b\overline{v_{*a}(x,z)}, \alpha_a\overline{v_{*b}(x,z)}\right)\xi \\ &= \frac{1}{W(\overline{z})} \left(-\alpha_b v_a(x,\overline{z}), \alpha_a v_b(x,\overline{z})\right)\xi, \end{aligned} \tag{2.17}$$

where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^a \end{pmatrix} \in \mathbb{C}^2. \tag{2.18}$$

The characteristic function Θ_H of the maximal dissipative operator H is a two-by-two matrix-valued function which satisfies the relation

$$\Theta_H(z)T(z)f = T_*(z)f, \quad z \in \varrho(H) \cap \varrho(H^*), \tag{2.19}$$

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

$$\|\Theta_H(z)\| \leq 1 \quad \text{for} \quad z \in \mathbb{C}_-. \tag{2.20}$$

Using the elementary solutions the characteristic function Θ_H takes the form

$$\Theta_H(z) = I_{\mathbb{C}^2} + i\frac{1}{W_*(z)} \begin{pmatrix} \alpha_b^2 v_{*a}(b,z) & -\alpha_b\alpha_a \\ -\alpha_b\alpha_a & \alpha_a^2 v_{*b}(a,z) \end{pmatrix}. \tag{2.21}$$

for $z \in \varrho(H) \cap \varrho(H^*)$, cf. [12]

Since H is a maximal dissipative operator there is a larger Hilbert space $\mathfrak{K} \supseteq \mathfrak{H}$ and a self-adjoint operator K on $\mathfrak{K}$ such that

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K - z)^{-1}|\mathfrak{H} = (H - z)^{-1}, \quad \Im\mathrm{m}(z) > 0, \tag{2.22}$$

see [8]. The operator K is called a self-adjoint dilation of the maximal dissipative operator H. Obviously, from the condition (2.22) one gets

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K - z)^{-1}|\mathfrak{H} = (H^* - z)^{-1}, \quad \Im\mathrm{m}(z) < 0. \tag{2.23}$$

K is called a minimal self-adjoint dilation of H if the condition

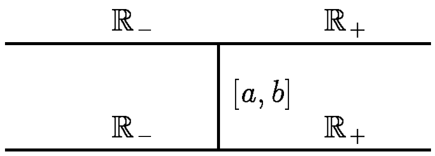
$$\bigvee_{z \in \mathbb{C}\setminus\mathbb{R}} (K - z)^{-1}\mathfrak{H} = \mathfrak{K} \tag{2.24}$$

is satisfied. 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. Following [12] we introduce the larger Hilbert space

$$\mathfrak{K} = \mathcal{D}_- \oplus \mathfrak{H} \oplus \mathcal{D}_+, \tag{2.25}$$

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



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

$$\vec{g} := g_- \oplus g \oplus g_+, \tag{2.26}$$

where

$$g_-(x) := \begin{pmatrix} g^b_-(x) \\ g^a_-(x) \end{pmatrix} \qquad \text{and} \quad g_+(x) := \begin{pmatrix} g^b_+(x) \\ g^a_+(x) \end{pmatrix}, \tag{2.27}$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively. Let the matrices $K^a_\pm$ and $K^b_\pm$ given by

$$K^a_- := \frac{1}{\alpha_a}\begin{pmatrix} 0 & 0 \\ 1 & \kappa_a \end{pmatrix} \qquad \text{and} \qquad K^a_+ := \frac{1}{\alpha_a}\begin{pmatrix} 0 & 0 \\ 1 & \overline{\kappa_a} \end{pmatrix} \tag{2.28}$$

as well as

$$K^b_- := \frac{1}{\alpha_b}\begin{pmatrix} 1 & -\kappa_b \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad K^b_+ := \frac{1}{\alpha_b}\begin{pmatrix} 1 & -\overline{\kappa_b} \\ 0 & 0 \end{pmatrix}. \tag{2.29}$$

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

$$\mathrm{dom}(K) := \left\{ \vec{g} \in \mathfrak{K} : \begin{array}{c} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2), \\ g, \frac{1}{m} g' \in W^{1,2}([a,b]), \\ K_-^a g_a + K_-^b g_b = g_-(0), \\ K_+^a g_a + K_+^b g_b = g_+(0) \end{array} \right\} \tag{2.30}$$

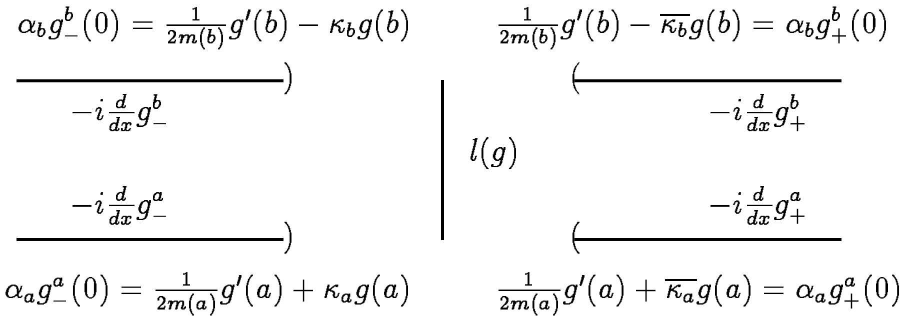
and

$$K\vec{g} := -i\frac{d}{dx} g_- \oplus l(g) \oplus -i\frac{d}{dx} g_+, \qquad \vec{g} \in \mathrm{dom}(K), \tag{2.31}$$

where

$$g_a = \begin{pmatrix} \frac{1}{2m(a)} g'(a) \\ g(a) \end{pmatrix} \quad \text{and} \quad g_b = \begin{pmatrix} \frac{1}{2m(b)} g'(b) \\ g(b) \end{pmatrix}. \tag{2.32}$$

With respect to a graph picture the operator K looks like



The self-adjoint operator K is absolutely continuous and its spectrum coincides with the real axis, i.e. $\sigma(K) = \mathbb{R}$. The multiplicity of its spectrum is two. The resolvent of K admits the representation

$$\begin{aligned} &(K - z)^{-1}(f_- \oplus f \oplus f_+) = \\ &i\int_{-\infty}^{x} dy\; e^{i(x-y)z} f_-(y) \;\oplus\; (H - z)^{-1} f + iT_*(\overline{z})^* \int_{-\infty}^{0} dy\; e^{-iyz} f_-(y) \;\oplus \\ &i\int_{0}^{x} dy\; e^{i(x-y)z} f_+(y) + ie^{izx} T(z) f + i\Theta_H(\overline{z})^* \int_{-\infty}^{0} dy\; e^{i(x-y)z} f_-(y) \end{aligned} \tag{2.33}$$

for $\Im\mathrm{m}(z) > 0$ and

$$\begin{aligned} &(K - z)^{-1}(f_- \oplus f \oplus f_+) = \\ &-i\int_{x}^{0} dy\; e^{i(x-y)z} f_-(y) - ie^{izx} T_*(z) f - i\Theta_H(z) \int_{0}^{\infty} dy\; e^{i(x-y)z} f_+(y) \oplus \\ &(H^* - z)^{-1} f - iT(\overline{z})^* \int_{0}^{\infty} dy\; e^{-iyz} f_+(y) \;\oplus\; -i\int_{x}^{\infty} dy\; e^{i(x-y)z} f_+(y) \end{aligned} \tag{2.34}$$

for $\Im\mathrm{m}(z) < 0$. The generalized eigenfunctions $\vec{\psi}^-(\cdot, \lambda, \tau)$, $\lambda \in \mathbb{R}$, $\tau = a, b$, of K are given by

$$\begin{aligned} &\vec{\psi}^-(x, \lambda, \tau) := \psi_-^-(x, \lambda, \tau) \oplus \psi^-(x, \lambda, \tau) \oplus \psi_+^-(x, \lambda, \tau) = \\ &\qquad \frac{1}{\sqrt{2\pi}} e^{ix\lambda} e_\tau \oplus \frac{1}{\sqrt{2\pi}} (T_*(\lambda)^* e_\tau)(x) \oplus \frac{1}{\sqrt{2\pi}} e^{ix\lambda} \Theta_H(\lambda)^* e_\tau \end{aligned} \tag{2.35}$$

where

$$e_b := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad e_a := \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.36}$$

The functions are mutually orthogonal, i.e. one has

$$\left(\vec{\psi}^-(\cdot,\lambda,\tau), \vec{\psi}^-(\cdot,\lambda',\tau')\right)_{L^2(\hat{\Omega})} = \delta(\lambda-\lambda')\delta_{\tau\tau'}, \tag{2.37}$$

in the sense of distribution for $\lambda, \lambda' \in \mathbb{R}$, $\tau, \tau' = a, b$. Moreover, elements of the form

$$\int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}^-(\cdot,\lambda,\tau)\hat{g}^\tau(\lambda) \tag{2.38}$$

where $\hat{g}^\tau(\cdot)$, $\tau = a, b$, are smooth functions with compact support, are dense in $\mathfrak{K}$. We note that the generalized eigenfunctions $\vec{\psi}^-(\cdot,\lambda,\tau)$ are usually called the incoming eigenfunctions. Using the incoming eigenfunctions one defines a transformation $\Phi_- : \mathfrak{K} \longrightarrow \hat{\mathfrak{K}} = L^2(\mathbb{R}, \mathbb{C}^2)$

$$(\Phi_- \vec{g})(\lambda) =: \hat{g}(\lambda) = \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix}, \tag{2.39}$$

where

$$\hat{g}^\tau(\lambda) := \int_{\hat{\Omega}} dx \left(\vec{g}(x), \vec{\psi}^-(x,\lambda,\tau)\right), \quad \tau = a, b. \tag{2.40}$$

Φ_- is unitary and called the incoming Fourier transformation. The inverse incoming Fourier transformation Φ_-^{-1} is given by

$$(\Phi_-^{-1}\hat{g})(x) = \int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}^-(x,\lambda,\tau)\hat{g}^\tau(\lambda), \quad \hat{g} \in L^2(\mathbb{R}, \mathbb{C}^2). \tag{2.41}$$

We note that

$$\Phi_- K \Phi_-^{-1} = M \tag{2.42}$$

where M is the multiplication operator by the independent variable λ on $\hat{\mathfrak{K}}$, i.e.

$$\begin{aligned} \mathrm{dom}(M) &:= \left\{\hat{g} \in L^2(\mathbb{R}, \mathbb{C}^2) : \lambda\hat{g}(\lambda) \in L^2(\mathbb{R}, \mathbb{C}^2)\right\}, \\ (M\hat{g})(\lambda) &:= \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathrm{dom}(M). \end{aligned} \tag{2.43}$$

The representation (2.43) induced by Φ_- is called the incoming spectral representation of K.

Finally, we note that each bounded self-adjoint operator G on $\mathfrak{K}$, which commutes with K, corresponds to a measurable family $\{G(\lambda)\}_{\lambda\in\mathbb{R}}$ of two-by-two matrices, which are uniformly bounded, i.e., $G(\cdot) \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$, such that the multiplication operator $\hat{G}$ on $L^2(\mathbb{R}, \mathbb{C}^2)$ defined by

$$\begin{aligned} \mathrm{dom}(\hat{G}) &:= \left\{\hat{g} \in L^2(\mathbb{R}, \mathbb{C}^2) : G(\lambda)\hat{g}(\lambda) \in L^2(\mathbb{R}, \mathbb{C}^2)\right\}, \\ (\hat{G}\hat{g})(\lambda) &:= G(\lambda)\hat{g}(\lambda), \quad \hat{g} \in \mathrm{dom}(\widehat{G(\cdot)}) \end{aligned} \tag{2.44}$$

is unitarily equivalent to G, i.e.

$$\Phi_- G \Phi_-^{-1} = \hat{G}. \tag{2.45}$$

Indeed, if G commutes with K, then $\hat{G}$ commutes with M. Applying Theorem VII.2.3 of [3] one immediately gets that $\hat{G}$ is a multiplication operator of type (2.44). The representation (2.44) is called the incoming spectral representation of G.

3 Carrier density

In the following we call an operator $\varrho : \mathfrak{K} \longrightarrow \mathfrak{K}$ a density matrix if ϱ is a bounded, non-negative operator. The operator ϱ is called a steady state if ϱ commutes with K. Obviously, a steady state does not change in time. If ϱ is a steady state, then there is a measurable matrix-valued function $\varrho(\cdot) \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that the multiplication operator $\hat{\varrho}$ on $L^2(\mathbb{R}, \mathbb{C}^2)$ generated by $\varrho(\cdot)$ is unitarily equivalent to ϱ, i.e.

$$\varrho = \Phi_-^{-1} \hat{\varrho} \Phi_-, \tag{3.1}$$

see above. Obviously, the measurable function $\varrho(\cdot)$ takes the form

$$\varrho(\lambda) = \begin{pmatrix} \varrho^{bb}(\lambda) & \varrho^{ba}(\lambda) \\ \varrho^{ab}(\lambda) & \varrho^{aa}(\lambda) \end{pmatrix} \tag{3.2}$$

where $\varrho^{\tau\nu}(\cdot) \in L^\infty(\mathbb{R})$, $\tau, \nu = a, b$. Since $\varrho \geq 0$ one gets that $\varrho(\lambda) \geq 0$ a.e. (with respect to the Lebesgue measure).

Definition 3.1 A bounded self-adjoint operator A on $\mathfrak{K}$ is called an observable. We say the observable A

(i) is admissible with respect to ϱ if ϱA is a nuclear operator on $\mathfrak{K}$, i.e. $\varrho A \in \mathcal{L}_1(\mathfrak{K})$,

(ii) is admissible with respect to K if $E_K(\Delta)A \in \mathcal{L}_1(\mathfrak{K})$ for each bounded interval $\Delta \subseteq \mathbb{R}$ where $E_K(\cdot)$ denotes the spectral measure of K.

If the observable A is admissible with respect to ϱ, then its expectation value $\mathbb{E}_\varrho(A)$ with respect to the density matrix ϱ is defined by

$$\mathbb{E}_\varrho(A) := \mathrm{tr}(\varrho A). \tag{3.3}$$

In the following we show that the admissibility of A with respect to K leads to a certain localization in the incoming spectral representation:

Proposition 3.2 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. If the observable A is admissible with respect to K, then there exists a measurable* *matrix-valued function* $A(\cdot) \in L^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$, *such that* $A(\lambda) = A(\lambda)^*$ *for a.e.* $\lambda \in \mathbb{R}$ *and*

$$\mathrm{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)A(\lambda)) \tag{3.4}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$ *and any steady state* ϱ *of* K. *The measurable function* $A(\cdot)$ *is uniquely defined up to a Borel set of Lebesgue measure zero.*

If the observable A *is in addition admissible with respect to the steady state* ϱ, *then* $\mathrm{tr}_{\mathbb{C}^2}(\varrho(\cdot)A(\cdot)) \in L^1(\mathbb{R})$ *and the representation*

$$\mathrm{tr}(\varrho A) = \int_{\mathbb{R}} d\lambda \ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)A(\lambda)) \tag{3.5}$$

holds.

Proof. Notice that the spectral measure $E_K(\cdot)$ of K is absolutely continuous with respect to Lebesgue measure. Hence, the set function

$$\mu_{\varrho,A}(\Delta) := \mathrm{tr}(\varrho A E_K(\Delta)), \tag{3.6}$$

where Δ is bounded Borel set of $\mathbb{R}$, is in fact a Lebesgue absolutely continuous measure. Let $\frac{d\mu_{\varrho,A}}{d\lambda}$ denote its Radon-Nikodym derivative and define

$$T_A(\hat{\varrho}) := \frac{d\mu_{\varrho,A}}{d\lambda}. \tag{3.7}$$

Then $T_A(\cdot)$ maps $L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ continuously into $L^1_{loc}(\mathbb{R})$ (the latter in its canonic Frechet topology) and, additionally, one has

$$\mathrm{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \ \frac{d\mu_{\varrho,A}}{d\lambda}(\lambda) = \int_\Delta d\lambda \ T_A(\hat{\varrho})(\lambda) \tag{3.8}$$

for any bounded Borel set $\Delta \subset \mathbb{R}$. It is not hard to see that (3.8) implies the equality

$$T_A(\chi_\Delta \hat{\varrho}) = \chi_\Delta T_A(\hat{\varrho}) \tag{3.9}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$ where χ_Δ denotes its indicator function. We put

$$e_{bb} := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \ e_{ba} := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \ e_{ab} := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \ e_{aa} := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.10}$$

and define for any $h \in L^\infty(\mathbb{R})$

$$A_{ij}(h) := T_A(h \cdot e_{ji}), \qquad i,j = a,b. \tag{3.11}$$

Clearly, each of the mappings $A_{ij}(\cdot)$ then maps $L^\infty(\mathbb{R})$ continuously into $L^1_{loc}(\mathbb{R})$ and (3.11) implies

$$A_{ij}(\chi_\Delta h) = \chi_\Delta A_{ij}(h) \tag{3.12}$$

for any $h \in L^\infty(\mathbb{R})$ and any Borel set Δ. Taking in particular $h \equiv 1$, this yields

$$A_{ij}(\chi_\Delta) = \chi_\Delta A_{ij}(1). \tag{3.13}$$

Obviously, by the linearity of the mappings $A_{ij}(\cdot)$, this last equation remains true if χ_Δ is there replaced by any (finite) linear combination of indicator functions. Because the set of finite linear combinations of indicator functions is dense in $L^\infty(\mathbb{R})$, one gets for all $h \in L^\infty(\mathbb{R})$ the equation

$$A_{ij}(h) = h \cdot A_{ij}(1). \tag{3.14}$$

Since

$$\varrho(\cdot) = \varrho^{bb}(\cdot)e_{bb} + \varrho^{ba}(\cdot)e_{ba} + \varrho^{ab}(\cdot)e_{ab} + \varrho^{aa}(\cdot)e_{aa} \tag{3.15}$$

one gets

$$\begin{gathered}\operatorname{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda\ T_A(\hat{\varrho})(\lambda) = \\ \sum_{i,j=a,b} \int_\Delta d\lambda\ A_{ij}(\varrho^{ij})(\lambda) = \sum_{i,j=a,b} \int_\Delta d\lambda\ \varrho^{ij}(\lambda) A_{ji}(1)(\lambda).\end{gathered} \tag{3.16}$$

Setting

$$A(\cdot) := \begin{pmatrix} A_{bb}(1)(\cdot) & A_{ba}(1)(\cdot) \\ A_{ab}(1)(\cdot) & A_{aa}(1)(\cdot) \end{pmatrix} \tag{3.17}$$

we finally obtain (3.4) for any bounded Borel set $\Delta \subset \mathbb{R}$ and any steady state ϱ of K.

Assume that $\tilde{A}(\cdot)$ obeys also the conditions of the proposition. Setting $G(\lambda) := A(\lambda) - \tilde{A}(\lambda)$, $\lambda \in \mathbb{R}$, one gets that

$$\int_\Delta \operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda)G(\lambda)) = 0 \tag{3.18}$$

for any bounded Borel set Δ and any steady state ϱ. Hence $\operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda)G(\lambda)) = 0$ for a.e. λ and any steady state ϱ which immediately yields $G(\lambda) = 0$ or $A(\lambda) = \tilde{A}(\lambda)$ for a.e. $\lambda \in \mathbb{R}$.

If ϱ is admissible with respect to A, then $|\operatorname{tr}(\varrho A E_K(\Delta)| < \|\varrho A\|_{\mathcal{L}_1}$ for any Borel set $\Delta \subseteq \mathbb{R}$. By (3.4) this implies that $\operatorname{tr}(\varrho(\cdot)A(\cdot)) \in L^1(\mathbb{R})$. Since one has $\lim_{\Delta\uparrow\mathbb{R}} \operatorname{tr}(\varrho A E_K(\Delta)) = \operatorname{tr}(\varrho A)$ we obtain from (3.4) the equality (3.5). □

Proposition 3.2 says that the averaging procedure localizes with respect to the incoming spectral representation. Indeed, the quantity $\operatorname{tr}(\varrho(\lambda)A(\lambda))$ can be regarded as the local average of the observable $A(\lambda)$ with respect to the density matrix $\varrho(\lambda)$ at energy $\lambda \in \mathbb{R}$, i.e.

$$\mathbb{E}_{\varrho(\lambda)}(A(\lambda)) := \operatorname{tr}(\varrho(\lambda)A(\lambda)). \tag{3.19}$$

Formula (3.5) has the meaning that the total average $\mathbb{E}_\varrho(A)$ is the sum of the local averages $\mathbb{E}_{\varrho(\lambda)}(A(\lambda))$, i.e.

$$\mathbb{E}_\varrho(A) = \int_\mathbb{R} d\lambda\ \mathbb{E}_{\varrho(\lambda)}(A(\lambda)). \tag{3.20}$$

Proposition 3.2 gives rise to the following

Definition 3.3 Let A be an observable which is admissible with respect to K. An element $A(\cdot) \in L^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ is called a localizer of A with respect to K if $A(\lambda)^* = A(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ and

$$\operatorname{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \, \operatorname{tr}(\varrho(\lambda) A(\lambda)) \tag{3.21}$$

holds for any bounded Borel subset $\Delta \subseteq \mathbb{R}$ and any steady state ϱ.

Proposition 3.2 says that an observable which is admissible with respect to K has always a unique localizer.

To calculate the carrier density we consider the observable $U(\omega)$, $\omega \subseteq \Omega$, given by

$$(U(\omega)\vec{f}\,)(x) = 0 \oplus \chi_\omega(x) f(x) \oplus 0, \quad \vec{f} \in L^2(\hat{\Omega}), \tag{3.22}$$

for any Borel subset $\omega \subseteq \Omega$. We note that the observable $U(\omega)$ is a projection on $\mathfrak{K}$ with $\operatorname{ran}(U(\omega)) \subseteq \mathfrak{H}$. Loosely speaking, the projection acts in fact only on the subspace $\mathfrak{H} \subseteq \mathfrak{K}$.

Lemma 3.4 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then for any Borel set $\omega \subseteq \Omega$ the observable $U(\omega)$ is admissible with respect to the minimal self-adjoint dilation K of the maximal dissipative operator H. If the steady state ϱ satisfies the condition*

$$C_{\hat{\varrho}} := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2 + 1} \|\varrho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty, \tag{3.23}$$

then for any Borel set $\omega \subseteq \Omega$ the observable $U(\omega)$ is admissible with respect to ϱ.

Proof. The relation (2.33) implies

$$U(\omega)(K - z)^{-1}\vec{f} = 0 \oplus \chi_\omega (H - z)^{-1} f + i\chi_\omega T_*(\overline{z})^* \int_{-\infty}^0 dy \, e^{-iyz} f_-(y) \; \oplus 0 \tag{3.24}$$

for $\vec{f} \in \mathfrak{K}$ and $z \in \mathbb{C}_+$. By Theorem 3.1 of [11] one gets that $(H - z)^{-1}$ is a trace class operator for each $z \in \mathbb{C}_+$. Hence $U(\omega)(H - z)^{-1}$ is a trace class operator for each $\omega \subseteq \Omega$. Since the operator $T_*(\overline{z})^*$ acts from the two dimensional Hilbert space $\mathbb{C}^2$ into $\mathfrak{H}$ one easily gets that the second addend of (3.24) is a trace class operator, too. Hence $U(\omega)(K - z)^{-1} \in \mathcal{L}_1(\mathfrak{K})$ for each Borel set $\omega \subseteq \Omega$ and $z \in \mathbb{C}_+$. Using the representation

$$U(\omega)E_K(\Delta) = U(\omega)(K - z)^{-1}(K - z)E_K(\Delta), \quad z \in \mathbb{C}_+, \tag{3.25}$$

we find that $U(\omega)E_K(\Delta)$ is a trace class operator for each Borel sets $\omega \subseteq \Omega$ and each bounded interval $\Delta \subseteq \mathbb{R}$. Hence, the observable $U(\omega)$ is admissible with respect to K for each Borel set $\omega \subseteq \Omega$.

Moreover, taking into account (3.23) and the representation

$$U(\omega)\,\varrho = U(\omega)(K-i)^{-1}(K-i)\varrho \tag{3.26}$$

one immediately gets that $U(\omega)\,\varrho$ is a trace class operator for each $\omega \subseteq \Omega$, because $(K-i)\varrho$ is bounded. Hence, $\varrho\, U(\omega)$ is a trace class operator for each Borel set $\omega \subseteq \Omega$ which yields that $U(\omega)\,\varrho$ is admissible with respect to ϱ □

Since $U(\omega)$ is admissible with respect to K for any Borel set $\omega \subseteq \Omega$ by Proposition 3.2 there is a unique localizer $U(\omega)(\cdot) : \mathbb{R} \longrightarrow \mathcal{B}(\mathbb{C}^2)$. We are going to calculate this localizer.

Proposition 3.5 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then for any Borel set $\omega \subseteq \Omega$ the localizer of $U(\omega)(\cdot)$ of the observable $U(\omega)$ is given by*

$$U(\omega)(\lambda) = \int_\omega dx\; D(x,\lambda) \tag{3.27}$$

where

$$D(x,\lambda) := \begin{pmatrix} |\psi^-(x,\lambda,b)|^2 & \psi^-(x,\lambda,a)\overline{\psi^-(x,\lambda,b)} \\ \psi^-(x,\lambda,b)\overline{\psi^-(x,\lambda,a)} & |\psi^-(x,\lambda,a)|^2 \end{pmatrix} \tag{3.28}$$

$x \in \Omega$, $\lambda \in \mathbb{R}$.

If the steady state ϱ satisfies the condition (3.23), then

$$\mathbb{E}_\varrho(U(\omega)) = \int_{\mathbb{R}} d\lambda\; \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\,U(\omega)(\lambda)) \tag{3.29}$$

for any Borel subset $\omega \subseteq \Omega$.

Proof. By Lemma 3.4 the observable $U(\omega)$ is admissible for any Borel set $\omega \subseteq \Omega$. By Proposition 3.2 there is a unique localizer $U(\omega)(\cdot) \in \mathcal{L}^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that (3.21) is satisfied for any bounded Borel set $\Delta \subseteq \mathbb{R}$ and any steady state ϱ. Following the proof of Proposition 3.2 we consider the measure

$$\mu_{\varrho,U(\omega)}(\Delta) = \mathrm{tr}(\varrho\, U(\omega) E_K(\Delta)) \tag{3.30}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$. We set $\hat{U}(\omega) := \Phi_- U(\omega)\Phi_-^{-1}$ and $\hat{U}_\Delta(\omega) := E_M(\Delta)\hat{U}E_M(\Delta)$ where $M = \Phi_- K \Phi_-^{-1}$, see (2.42). By Lemma 3.4 the operator $\hat{U}_\Delta(\omega)$ is nuclear. Hence, we find

$$\mu_{\varrho,U(\omega)}(\Delta) = \mathrm{tr}(\hat{\varrho}\,\hat{U}_\Delta(\omega)). \tag{3.31}$$

Let us calculate the kernel of $\hat{U}_\Delta(\omega)$. To his end we consider the scalar product $(\hat{U}_\Delta(\omega)\hat{g}, \hat{f})$, $\hat{g}, \hat{f} \in L^2(\Delta, \mathbb{C}^2)$. Using (2.41) one has

$$(\hat{U}_\Delta(\omega)\hat{g},\hat{f}) = \tag{3.32}$$
$$\int_\omega dx \int_\Delta d\lambda \sum_{\tau=a,b} \psi^-(x,\lambda,\tau)\hat{g}^\tau(\lambda)\overline{\int_\Delta d\mu \sum_{\xi=a,b} \psi^-(x,\mu,\xi)\hat{f}^\xi(\mu)}.$$

Setting

$$U_\Delta^{\tau\xi}(\omega)(\mu,\lambda) := \int_\omega dx\, \psi^-(x,\lambda,\xi)\overline{\psi^-(x,\mu,\tau)}, \quad \tau,\xi = a,b, \tag{3.33}$$

we get

$$(\hat{U}_\Delta(\omega)\hat{g},\hat{f}) = \tag{3.34}$$
$$\int_\Delta d\mu \left(\int_\Delta d\lambda \begin{pmatrix} U_\Delta^{bb}(\omega)(\mu,\lambda) & U_\Delta^{ba}(\omega)(\mu,\lambda) \\ U_\Delta^{ab}(\omega)(\mu,\lambda) & U_\Delta^{aa}(\omega)(\mu,\lambda) \end{pmatrix} \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix}, \begin{pmatrix} \hat{f}^b(\mu) \\ \hat{f}^a(\mu) \end{pmatrix}\right)$$

what shows that

$$U_\Delta(\omega)(\mu,\lambda) := \begin{pmatrix} U_\Delta^{bb}(\omega)(\mu,\lambda) & U_\Delta^{ba}(\omega)(\mu,\lambda) \\ U_\Delta^{ab}(\omega)(\mu,\lambda) & U_\Delta^{aa}(\omega)(\mu,\lambda) \end{pmatrix} \tag{3.35}$$

is the kernel of the integral operator $\hat{U}_\Delta(\omega)$. Setting

$$D(x,\mu,\lambda) := \begin{pmatrix} \psi^-(x,\lambda,b)\overline{\psi^-(x,\mu,b)} & \psi^-(x,\lambda,a)\overline{\psi^-(x,\mu,b)} \\ \psi^-(x,\lambda,b)\overline{\psi^-(x,\mu,a)} & \psi^-(x,\lambda,a)\overline{\psi^-(x,\mu,a)} \end{pmatrix} \tag{3.36}$$

we obtain the representation

$$U_\Delta(\omega)(\mu,\lambda) = \int_\omega dx\, D(x,\mu,\lambda),\ \mu,\lambda \in \Delta. \tag{3.37}$$

Since $U_\Delta(\omega)(\mu,\lambda) = U_{\Delta'}(\omega)(\mu,\lambda)$ for $\mu,\lambda \in \Delta \subseteq \Delta'$ it makes sense to define $U(\omega)(\mu,\lambda) := \lim_{\Delta\uparrow\mathbb{R}} U_\Delta(\omega)(\mu,\lambda)$, $\mu,\lambda\in\mathbb{R}$. Hence $U_\Delta(\omega)(\mu,\lambda) = U(\omega)(\mu,\lambda)$ for $\mu,\lambda\in\Delta$ and

$$U(\omega)(\mu,\lambda) = \int_\omega dx\, D(x,\mu,\lambda), \quad \mu,\lambda\in\Delta. \tag{3.38}$$

Since the kernel depends continuously on μ and λ one gets that

$$\mathrm{tr}(\hat{\varrho}\,\hat{U}_\Delta(\omega)) = \int_\Delta d\lambda\, \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\, U(\omega)(\lambda,\lambda)) \tag{3.39}$$

for any bounded Borel set $\Delta\subseteq\mathbb{R}$ and any steady state ϱ. From (3.38) we find that $U(\omega)(\lambda,\lambda)^* = U(\omega)(\lambda,\lambda)$ for $\lambda\in\mathbb{R}$. Since the eigenfunctions $\psi^-(x,\lambda,b)$ and $\psi^-(x,\lambda,a)$ are bounded on compact sets of x and λ we obtain that $U(\omega)(\lambda,\lambda) \in L^1_{loc}(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$. By (3.39) the matrix-valued function $U(\omega)(\lambda) := U(\omega)(\lambda,\lambda)$, $\lambda\in\mathbb{R}$, is the unique localizer of the observable $U(\omega)$. By condition (3.23) the observable $U(\omega)$ is admissible with respect to ϱ. Applying Proposition 3.2 we verify (3.29).

It remains to verify (3.27) and (3.28). From (3.38) and (3.39) we obtain the representation

$$\mathrm{tr}(\hat{\varrho}\,\hat{U}_\Delta(\omega)) = \int_\Delta d\lambda \int_\omega dx\, \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\, D(x,\lambda,\lambda)). \tag{3.40}$$

Setting $D(x,\lambda) := D(x,\lambda,\lambda)$, $x\in\Omega$. $\lambda\in\mathbb{R}$, we immediately obtain (3.27) and (3.28). □

We set

$$u_{\hat{\varrho}}(x,\lambda) := \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)\; D(x,\lambda)\right) \tag{3.41}$$

for $x \in \Omega$ and $\lambda \in \mathbb{R}$. A simple computation shows that the eigenvalues of $D(x,\lambda)$ are equal to $|\psi^-(x,\lambda,b)|^2$ and $|\psi^-(x,\lambda,a)|^2$ which shows that the matrix $D(x,\lambda)$ is non-negative for each $x \in \Omega$ and $\lambda \in \mathbb{R}$. Since for a.e. $\lambda \in \mathbb{R}$ the matrix $\varrho(\lambda)$ is non-negative, too one gets that $u_{\hat{\varrho}}(x,\lambda) \geq 0$ for $x \in \Omega$ and a.e. $\lambda \in \mathbb{R}$. This fact can also be verified taking into account the representation

$$u_{\hat{\varrho}}(x,\lambda) = \left\langle \varrho^t(\lambda) \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle \tag{3.42}$$

where $\varrho^t(\lambda)$ is the transposed matrix to (3.2). Moreover, if condition (3.23) is satisfied, then from Proposition (3.5) we obtain the representation

$$\mathbb{E}_\varrho(U(\omega)) = \int_{\mathbb{R}} d\lambda \int_\omega dx\; u_{\hat{\varrho}}(x,\lambda) \tag{3.43}$$

for Borel sets $\omega \subseteq \Omega$. Taking into account Fubini's theorem we find that

$$\mathbb{E}_\varrho(U(\omega)) = \int_\omega dx\; u_{\hat{\varrho}}(x). \tag{3.44}$$

where

$$u_{\hat{\varrho}}(x) := \int_{\mathbb{R}} d\lambda\; u_{\hat{\varrho}}(x,\lambda) \geq 0, \quad x \in \Omega, \tag{3.45}$$

and $u_{\hat{\varrho}} \in L^1(\Omega)$. The representation (3.44) shows that $\mathbb{E}_\varrho(U(\cdot))$ defines a measure on Ω which is absolutely continuous with respect to the Lebesgue measure. Since the expectation value $\mathbb{E}_\varrho(U(\omega))$ has the meaning of the number of carriers in $\omega \subseteq \Omega$ its Radon-Nikodym derivative can be interpreted as the carrier density of the system described by K and mutatis mutandis by H.

Definition 3.6 Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then the matrix $D(x,\lambda)$, $x \in \Omega$, and the value $u_{\hat{\varrho}}(x,\lambda)$ are called carrier density observable and carrier density at $x \in \Omega$ and at energy $\lambda \in \mathbb{R}$ of the system described by H, respectively.

This definition is justified by the fact that by (3.41) the carrier density $u_{\hat{\varrho}}(x,\lambda)$ is the expectation value of the carrier density observable $D(x,\lambda)$, i.e. $u_{\hat{\varrho}}(x,\lambda) = \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda))$ at $x \in \Omega$ and at $\lambda \in \mathbb{R}$. Moreover, we note that (3.45) can be written as

$$u_{\hat{\varrho}}(x) = \int_{\mathbb{R}} d\lambda\; \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)), \quad x \in \Omega, \tag{3.46}$$

i.e, the carrier density at $x \in \Omega$ is the sum of expectation values of the carrier density observable at $x \in \Omega$ over all energies.

On the Hilbert space $\mathfrak{K} = L^2(\hat{\Omega})$ we consider the multiplication operator $M(h)$,

$$(M(h)\vec{f})(x) = 0 \oplus h(x)f(x) \oplus 0, \quad x \in \Omega, \tag{3.47}$$

for real functions $h \in L^\infty(\Omega)$. We note that $M(\chi_\omega) = U(\omega)$ for any Borel set $\omega \subseteq \Omega$. In particular, one has $M(\chi_\Omega) = U(\Omega) = P_{\mathfrak{H}}^{\mathfrak{K}}$. Obviously, the representation

$$\varrho\, M(h) = \varrho\, U(\Omega)\, M(h), \quad h \in L^\infty(\Omega), \tag{3.48}$$

is valid. Since the observable $U(\Omega)$ is admissible with respect to ϱ the product $\varrho\, U(\Omega)$ is a nuclear operator on $\mathfrak{K}$ which yields that $\varrho M(h)$ is a nuclear operator on $\mathfrak{K}$, i.e. the observable $M(h)$ is admissible with respect to ϱ.

Proposition 3.7 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. If the steady state ϱ satisfies the condition (3.23), then the carrier density $u_{\hat\varrho}$ defined by (3.45) is a non-negative L^1-function such that*

$$\mathrm{tr}(\varrho M(h)) = \int_\Omega dx\; u_{\hat\varrho}(x) h(x) \tag{3.49}$$

for real functions $h \in L^\infty(\Omega)$. In particular, one has

$$\|u_{\hat\varrho}\|_{L^1(\omega)} = \mathrm{tr}(\varrho\, U(\omega)) \le C_{\hat\varrho} \|(K-i)^{-1} P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathcal{L}_1(\mathfrak{K})} \tag{3.50}$$

for each Borel set $\omega \subseteq \Omega$.

Proof. Setting $\omega = \Omega$ we obtain from (3.44) that $u_{\hat\varrho} \in L^1(\Omega)$. We choose $h = \chi_\omega$, $\omega \subseteq \Omega$. By (3.44) we get

$$\mathrm{tr}(\varrho M(\chi_\omega)) = \int_\Omega dx\; u_{\hat\varrho}(x)\chi_\omega(x). \tag{3.51}$$

By linearity this equation extends to

$$\mathrm{tr}(\varrho M(h)) = \int_\Omega dx\; u_{\hat\varrho}(x) h(x) \tag{3.52}$$

where h is an arbitrary step function on Ω. Since $u_{\hat\varrho}$ is from $L^1(\Omega)$ and $\varrho U(\Omega)$ is a nuclear operator both sides of (3.52) admit a continuation to L^∞-functions which verifies (3.49).

It remains to show the estimate (3.50). From (3.44) we immediately get

$$\int_\Omega dx\; u_g(x) = \mathrm{tr}(\varrho U(\Omega)) = \mathrm{tr}(\varrho(K-i)(K-i)^{-1}U(\Omega)). \tag{3.53}$$

Since $U(\Omega)(K-i)^{-1} \in \mathcal{L}_1(\mathfrak{K})$ and $\varrho(K-i)$ is a bounded operator which norm can be estimated by $C_{\hat\varrho}$ we obtain

$$\mathrm{tr}(\varrho(K-i)(K-i)^{-1}U(\omega)) \le C_{\hat\varrho}\|(K-i)^{-1}P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathcal{L}_1(\mathfrak{K})} \tag{3.54}$$

which verifies (3.50). □

Obviously, the relation (3.49) takes the form

$$\operatorname{tr}(\varrho M(h)) = \langle u_{\hat{\varrho}}, h\rangle_{L^1} \tag{3.55}$$

where by $\langle \cdot, h\rangle_{L^1}$, $h \in L^\infty(\Omega)$, we denote the linear functionals on $L^1(\Omega)$.

We conclude this section with some considerations which we need in the following section. Since $\{\varrho(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of non-negative self-adjoint operators there is a measurable family $\{V(\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary operators on $\mathbb{C}^2$ such that

$$\varrho(\lambda) = V(\lambda)\begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V(\lambda)^* \tag{3.56}$$

for a.e. $\lambda \in \mathbb{R}$ where $\mu_b(\lambda)$ and $\mu_a(\lambda)$ are the non-negative eigenvalues of $\varrho(\lambda)$. From (3.56) we get that

$$\varrho^t(\lambda) = V^t(\lambda)^*\begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V^t(\lambda) \tag{3.57}$$

for a.e. $\lambda \in \mathbb{R}$ where $V^t(\lambda)$ is the transposed matrix to $V(\lambda)$. Inserting (3.57) into (3.42) we obtain the expression

$$u_{\hat{\varrho}}(x,\lambda) = \tag{3.58}$$
$$\left\langle \begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix}, V^t(\lambda)\begin{pmatrix} \phi^-(x,\lambda,b) \\ \phi^-(x,\lambda,a)\end{pmatrix}\right\rangle.$$

Let us introduce the unit vectors $e_\tau(\lambda)$,

$$e_\tau(\lambda) = V(\lambda)e_\tau, \quad \tau = b, a \tag{3.59}$$

which perform an orthonormal basis in $\mathbb{C}^2$. We set

$$\vec{\psi}(x,\lambda,e_\tau(\lambda)) := \psi_-(x,\lambda,e_\tau(\lambda)) \oplus \psi(x,\lambda,e_\tau(\lambda)) \oplus \psi_+(x,\lambda,e_\tau(\lambda)) = \tag{3.60}$$
$$\frac{1}{\sqrt{2\pi}}e^{ix\lambda}e_\tau(\lambda) \oplus \frac{1}{\sqrt{2\pi}}(T_*(\lambda)^*e_\tau(\lambda))(x) \oplus \frac{1}{\sqrt{2\pi}}e^{ix\lambda}\Theta_H(\lambda)^*e_\tau(\lambda).$$

Obviously, the system $\{\vec{\psi}(x,\lambda,e_\tau(\lambda))\}_{\tau=b,a}$ performs an orthonormal basis of generalized eigenfunctions. Moreover, a straightforward computation shows that

$$V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix} = \begin{pmatrix} \psi(x,\lambda,e_b(\lambda)) \\ \psi(x,\lambda,e_a(\lambda))\end{pmatrix} \tag{3.61}$$

which leads to

$$u_{\hat{\varrho}}(x,\lambda) = \mu_b(\lambda)|\psi(x,\lambda,e_b(\lambda))|^2 + \mu_a(\lambda)|\psi(x,\lambda,e_a(\lambda))|^2 \tag{3.62}$$

for $x \in \Omega$ and $\lambda \in \mathbb{R}$.

4 Current density

In accordance with (1.11) the current density $j_{\hat{\varrho}}(x,\lambda)$ for the energy $\lambda \in \mathbb{R}$ is defined by

$$\begin{aligned} j_{\hat{\varrho}}(x,\lambda) \quad := \quad & \mu_b(\lambda)\Im\mathrm{m}\left(\tfrac{1}{m(x)}\psi(x,\lambda,e_b(\lambda))'\,\overline{\psi(x,\lambda,e_b(\lambda))}\right) + \\ & \mu_a(\lambda)\Im\mathrm{m}\left(\tfrac{1}{m(x)}\psi(x,\lambda,e_a(\lambda))'\,\overline{\psi(x,\lambda,e_a(\lambda))}\right) \end{aligned}, \tag{4.1}$$

$x \in \Omega$, where the eigenfunctions $\psi(x,\lambda,e_\tau(\lambda))$, $\tau = a,b$, are defined by (3.61). We are going to relate the current density to the characteristic function of the maximal dissipative operator H.

Proposition 4.1 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a,\kappa_b \in \mathbb{C}_+$. Further, let ϱ be a steady state. Then the current density $j_{\hat{\varrho}}(x,\lambda)$, $x\in\Omega$, $\lambda\in\mathbb{R}$, is independent from x and admits the representation*

$$j_{\hat{\varrho}}(\lambda) = \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)C(\lambda)\right) \tag{4.2}$$

where

$$C(\lambda) := -\frac{1}{2\pi i}\frac{\alpha_a\alpha_b}{\overline{W(\lambda)}}E\Theta_H(\lambda)^* = \frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}\Theta_H(\lambda)E, \tag{4.3}$$

$\lambda \in \mathbb{R}$. Moreover, if $\mathrm{tr}_{\mathbb{C}^2}(\varrho(\cdot)) \in L^1(\mathbb{R})$, then the total current $j_{\hat{\varrho}}$,

$$j_{\hat{\varrho}} := \int_{\mathbb{R}} d\lambda\; j_{\hat{\varrho}}(\lambda), \tag{4.4}$$

is finite and satisfies the estimate

$$|j_{\hat{\varrho}}| \le \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\; \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)\right) \tag{4.5}$$

Proof. From the definition (4.2) one gets that

$$j_{\hat{\varrho}}(x,\lambda) = \tag{4.6}$$
$$\Im\mathrm{m}\left(\left\langle\begin{pmatrix}\mu_b(\lambda) & 0\\ 0 & \mu_a(\lambda)\end{pmatrix}\begin{pmatrix}\frac{1}{m(x)}\psi(x,\lambda,e_b(\lambda))'\\ \frac{1}{m(x)}\psi(x,\lambda,e_a(\lambda))'\end{pmatrix},\begin{pmatrix}\psi(x,\lambda,e_b(\lambda))\\ \psi(x,\lambda,e_a(\lambda))\end{pmatrix}\right\rangle\right).$$

Taking into account (3.57) and (3.61) we get

$$j_{\hat{\varrho}}(x,\lambda) = \Im\mathrm{m}\left(\left\langle\varrho^t(\lambda)\begin{pmatrix}\frac{1}{m(x)}\psi^-(x,\lambda,b)'\\ \frac{1}{m(x)}\psi^-(x,\lambda,a)'\end{pmatrix},\begin{pmatrix}\psi^-(x,\lambda,b)\\ \psi^-(x,\lambda,a)\end{pmatrix}\right\rangle\right) \tag{4.7}$$

which can be expressed by

$$j_{\hat{\varrho}}(x,\lambda) = \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)C(x,\lambda)\right) \tag{4.8}$$

where

$$C(x,\lambda) := \tag{4.9}$$
$$\Im\mathrm{m}\left(\begin{pmatrix} \frac{1}{m(x)}\psi^-(x,\lambda,b)'\,\overline{\psi^-(x,\lambda,b)} & \frac{1}{m(x)}\psi^-(x,\lambda,a)'\,\overline{\psi^-(x,\lambda,b)} \\ \frac{1}{m(x)}\psi^-(x,\lambda,b)'\,\overline{\psi^-(x,\lambda,a)} & \frac{1}{m(x)}\psi^-(x,\lambda,a)'\,\overline{\psi^-(x,\lambda,a)} \end{pmatrix}\right)$$

We note that

$$C(x,\lambda) = \frac{1}{i}\begin{pmatrix} W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,b)) & W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,a)) \\ W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,b)) & W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,a)) \end{pmatrix} \tag{4.10}$$

where $W(\cdot,\cdot)$ is the Wronskian defined by (2.5). Since

$$W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,b)) = -\frac{i}{2\pi}\frac{\alpha_b^2\alpha_a^2}{|W(\lambda)|^2} \tag{4.11}$$

$$W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,b)) = \frac{1}{2\pi}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\left\{W(\lambda) - i\alpha_b^2 v_a(b,\lambda)\right\} \tag{4.12}$$

$$W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,a)) = -\frac{1}{2\pi}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\left\{W(\lambda) - i\alpha_a^2 v_b(a,\lambda)\right\} \tag{4.13}$$

$$W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,a)) = \frac{i}{2\pi}\frac{\alpha_a^2\alpha_b^2}{|W(\lambda)|^2} \tag{4.14}$$

we find

$$C(x,\lambda) = \frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\begin{pmatrix} -i\alpha_b\alpha_a & -(W(\lambda) - i\alpha_a^2 v_b(a,\lambda)) \\ W(\lambda) - i\alpha_b^2 v_a(b,\lambda) & i\alpha_a\alpha_b \end{pmatrix}. \tag{4.15}$$

This yields

$$C(x,\lambda) = \tag{4.16}$$
$$-\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} W(\lambda) - i\alpha_b^2 v_a(b,\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & W(\lambda) - i\alpha_a^2 v_b(a,\lambda) \end{pmatrix}.$$

From (2.21) we obtain

$$\Theta_H(\lambda)^* = \frac{1}{\overline{W(\lambda)}}\begin{pmatrix} W(\lambda) - i\alpha_b^2 v_a(b,\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & W(\lambda) - i\alpha_a^2 v_b(a,\lambda) \end{pmatrix}. \tag{4.17}$$

Hence, one has

$$C(x,\lambda) = -\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}E\Theta_H(\lambda)^* \tag{4.18}$$

where

$$E := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4.19}$$

This shows that $C(x,\lambda)$ is actually independent of $x \in \Omega$. By (4.8) this leads to the representation

$$j_{\hat{\varrho}}(x,\lambda) = -\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}\mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)E\Theta_H(\lambda)^*\right) \tag{4.20}$$

which shows that the current density is also independent of $x \in \Omega$. Thus it makes sense to denote $C(x,\lambda)$ and $j_{\hat{e}}(x,\lambda)$ by $C(\lambda)$ and $j_{\hat{e}}(\lambda)$, respectively. Hence, we have proved one part of the assertion (4.2) and (4.3). Taking into account the identity

$$\frac{1}{\overline{W(\lambda)}} E\Theta_H(\lambda)^* = -\frac{1}{W(\lambda)}\Theta_H(\lambda)E \tag{4.21}$$

we verify the other part.

It remains to show (4.4) and (4.5). To this end we note that from (4.17) one gets

$$J\Theta_H(\lambda)^* = J + \frac{i}{W(\lambda)}\begin{pmatrix} \alpha_b\alpha_a & -\alpha_a^2 v_b(a,\lambda) \\ -\alpha_b^2 v_a(b,\lambda) & \alpha_b\alpha_a \end{pmatrix} \tag{4.22}$$

where

$$J := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.23}$$

Hence we find

$$\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*) = 2i\frac{\alpha_b\alpha_a}{W(\lambda)} \tag{4.24}$$

which yields

$$\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)} = -\frac{1}{4\pi}\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*). \tag{4.25}$$

Using the definition (4.3) we finally obtain

$$j_{\hat{e}}(\lambda) = -\frac{1}{4\pi}\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*)\,\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\Theta_H(\lambda)E). \tag{4.26}$$

This leads to the estimate

$$|j_{\hat{e}}(\lambda)| \le \frac{1}{4\pi}\|\Theta_H(\lambda)^*\|_{\mathcal{L}_1(\mathbb{C}^2)}\|\varrho(\lambda)\|_{\mathcal{L}_1(\mathbb{C}^2)}. \tag{4.27}$$

Since $\|\Theta_H(\lambda)^*\|_{\mathcal{L}_1(\mathbb{C}^2)} \le 2$ and $\|\varrho(\lambda)\|_{\mathcal{L}_1(\mathbb{C}^2)} = \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda))$ we find

$$|j_{\hat{e}}(\lambda)| \le \frac{1}{2\pi}\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)) \tag{4.28}$$

which immediately proves (4.5). □

In correspondence to the carrier density it seems to be useful to introduce the following definition.

Definition 4.2 Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then the matrix $C(\lambda)$ and the value $j_\varrho(\lambda)$ are called the current density observable and the current density at energy $\lambda \in \mathbb{R}$ of the system described by H, respectively.

The definition is again justified by the fact that the current density at energy $\lambda \in \mathbb{R}$ is the expectation value of the current density observable at energy $\lambda \in \mathbb{R}$, i.e. $j_{\hat{\varrho}}(\lambda) = \mathbb{E}_{\varrho(\lambda)}(C(\lambda))$ for $\lambda \in \mathbb{R}$. Using this notation formula (4.4) takes the form

$$j_{\hat{\varrho}} = \int_{\mathbb{R}} d\lambda \; \mathbb{E}_{\varrho(\lambda)}(C(\lambda)). \tag{4.29}$$

In the following corollary we consider the case that the steady state ϱ is a function of K, i.e.

$$\varrho = f(K), \tag{4.30}$$

where, of course, $f(\cdot) \in L^\infty(\mathbb{R})$ and $f(\lambda) \geq 0$ for a.e. $\lambda \in \mathbb{R}$ and. In this case the density matrix ϱ belongs to the bicommutant of K.

Corollary 4.3 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. If the steady state ϱ is given by (4.30) with a non-negative function $f(\cdot) \in L^\infty(\mathbb{R})$, then $j_{\hat{\varrho}}(\lambda) = 0$ for a.e. $\lambda \in \mathbb{R}$.*

Proof. In this case one has

$$\varrho(\lambda) = f(\lambda) I_{\mathbb{C}^2}, \quad \lambda \in \mathbb{R}. \tag{4.31}$$

which gives

$$j_{\hat{\varrho}}(\lambda) = f(\lambda)\mathrm{tr}(C(\lambda)) = -\frac{1}{2\pi i} f(\lambda) \frac{\alpha_b \alpha_a}{W(\lambda)} \mathrm{tr}_{\mathbb{C}^2}(E\Theta_H(\lambda)^*). \tag{4.32}$$

By (4.17) we immediately get that $\mathrm{tr}_{\mathbb{C}^2}(E\Theta_H(\lambda)^*) = 0$ for $\lambda \in \mathbb{R}$. $\square$

If the steady state ϱ has the form

$$\varrho(\lambda) = \begin{pmatrix} \varrho^{bb}(\lambda) & 0 \\ 0 & \varrho^{aa}(\lambda) \end{pmatrix}, \tag{4.33}$$

then the current density is given by

$$j_{\hat{\varrho}}(\lambda) = -\frac{1}{2\pi} \frac{\alpha_a^2 \alpha_b^2}{|W(\lambda)|^2} (\varrho^{bb}(\lambda) - \varrho^{aa}(\lambda)). \tag{4.34}$$

This current density is different from zero if $\varrho^{bb}(\lambda) \neq \varrho^{aa}(\lambda)$ at least for a set of positive Lebesgue measure. So a current density different from zero arises only if we have a occupation disparity between the two eigenstates $\psi^-(x, \lambda, b)$ and $\psi^-(x, \lambda, a)$. This is the case if the steady state ϱ belongs to the commutant of K but not to the bicommutant. In other words, the density matrix (1.8) used for self-adjoint boundary conditions and generalized by (4.30) to the dissipative case leads to a zero current density.

5 Remarks

1. The carrier density $u_{\hat{\varrho}}(\cdot)$ performed by (3.41) and (3.44) is a straightforward generalization of the corresponding definition (1.5) of the carrier density in the self-adjoint case. Indeed, this correspondence relies on the replacements

$$\begin{array}{rcl} l & \longleftrightarrow & \{a, b, \lambda\}, \\ \{\psi_l\}_{l=1}^{\infty} & \longleftrightarrow & \{\vec{\psi}(\cdot, \lambda, \tau)\}_{\lambda \in \mathbb{R}, \tau = a,b}, \\ \sum_{l=1}^{\infty} & \longleftrightarrow & \int_{\lambda \in \mathbb{R}} d\lambda \, \sum_{\tau = a,b} \\ \varrho_l & \longleftrightarrow & \varrho(\lambda) \end{array} \tag{5.1}$$

The same holds for the current density defined by (4.1) which is a straightforward generalization of (1.11). *However, in contrast to the self-adjoint case the current density now is not necessarily zero!*

2. There is consensus in the conviction that scattering states are responsible for the current. This usually leads to a a relation between current density and scattering matrix. Actually, the same takes place here. Formulae (4.2) and (4.3) relate the current density $j_{\hat{\varrho}}(\lambda)$ with the characteristic function $\Theta_{H^*}(\lambda)$ of H^*. It turns out that the characteristic function $\Theta_{H^*}(\lambda)$ of H^* can be regarded as the scattering matrix of an associated scattering system. Indeed, with the self-adjoint dilation K one can associate a so-called Lax-Phillips scattering theory [2, 16]. To this end one introduces the Hilbert space $\mathfrak{K}_0$,

$$\mathfrak{K}_0 := L^2(\mathbb{R}, \mathbb{C}^2) = \mathcal{D}_- \oplus \mathcal{D}_+ \subseteq \mathfrak{K}. \tag{5.2}$$

and the identification operators $J_\pm : \mathfrak{K}_0 \longrightarrow \mathfrak{K}$,

$$\begin{array}{rcl} \vec{f} = J_- f & := & P^{\mathfrak{K}_0}_{\mathcal{D}_-} f \oplus 0 \oplus 0, \quad f \in \mathfrak{K}_0, \\ \vec{f} = J_+ f & := & 0 \oplus 0 \oplus P^{\mathfrak{K}_0}_{\mathcal{D}_+} f, \quad f \in \mathfrak{K}_0. \end{array} \tag{5.3}$$

The subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called incoming and outgoing subspaces, respectively. On the Hilbert space $\mathfrak{K}_0$ one defines the self-adjoint operator K_0,

$$(K_0 f)(x) = -i \frac{d}{dx} f(x) \tag{5.4}$$

with the domain $\mathrm{dom}(K_0) := W^{1,2}(\mathbb{R}, \mathbb{C}^2)$. The Lax-Phillips wave operators

$$W_\pm = s - \lim_{t \to \pm\infty} e^{itK} J_\pm e^{-itK_0} \tag{5.5}$$

exist and are complete, i.e. $\mathrm{ran}(W_\pm) = \mathfrak{K}$. The corresponding Lax-Phillips scattering operator $S = W_+^* W_- : \mathfrak{K}_0 \longrightarrow \hat{\mathfrak{K}}$, is unitary and commutes with the self-adjoint operator K_0. By $\mathcal{F} : \mathfrak{K}_0 \longrightarrow \hat{\mathfrak{K}}$ we denote the Fourier transform

$$(\mathcal{F} f)(\lambda) = \hat{f}(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx \; e^{-i\lambda x} f(x), \quad f \in \mathfrak{K}_0, \quad \lambda \in \mathbb{R}. \tag{5.6}$$

We note that $\mathcal{F}K_0\mathcal{F}^{-1} = M$ where M is defined by (2.43). Since S commutes with K_0 the operator $\hat{S} = \mathcal{F}S\mathcal{F}^{-1} : \hat{\mathfrak{K}} \longrightarrow \hat{\mathfrak{K}}$ commutes with M. Hence $\hat{S}$ is a multiplication operator given by

$$(\hat{S}\hat{f})(\lambda) = S(\lambda)\hat{f}(\lambda), \quad \hat{f} \in \hat{\mathfrak{K}}, \quad \lambda \in \mathbb{R}, \tag{5.7}$$

where $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of unitary operators which is called the Lax-Phillips scattering matrix. A rather involved computation shows that

$$S(\lambda) = \Theta_{H^*}(\lambda) \tag{5.8}$$

for a.e. $\lambda \in \mathbb{R}$, see for example [1]. By the way one has

$$\Phi_- = \mathcal{F}W_+^* \quad \text{and} \quad \Phi_+ = \mathcal{F}W_-^* \tag{5.9}$$

where is Φ_- is the incoming Fourier transformation, cf. (2.41) and (2.42), and Φ_+ is the so-called outgoing Fourier transform which was introduced in [12].

3. As mentioned above the quantity $N_\varrho(\omega)$,

$$N_\varrho(\omega) := \|u_{\hat{\varrho}}\|_{L^1(\omega)} = \int_\omega dx\; u_{\hat{\varrho}}(x), \tag{5.10}$$

has the meaning of the number of carriers on the Borel set subset $\omega \subseteq \Omega = [a, b]$. By (3.44) one has the representation

$$N_\varrho(\omega) = \operatorname{tr}(\varrho U(\omega)). \tag{5.11}$$

Obviously $N := N_\varrho(\Omega)$ is the total number of carriers on the interval $[a, b]$. We note that under the condition(3.23) by Proposition 3.7 the total number of carriers in Ω is always finite.

In accordance with [15] the time evolution of the density matrix ϱ is given by

$$\varrho(t) = e^{-itK}\varrho e^{itK}, \quad t \in \mathbb{R}. \tag{5.12}$$

Hence, the number of particles at time $t \in \mathbb{R}$ on ω is given by

$$N_{\varrho(t)}(\omega) := \operatorname{tr}(\varrho(t)U(\omega)), \quad t \in \mathbb{R}. \tag{5.13}$$

Since ϱ commutes with K one has $\varrho(t) = \varrho$ and $N_{\varrho(t)}(\omega) = N_\varrho(\omega)$ or

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = 0, \quad \omega \subseteq \Omega, \quad t \in \mathbb{R}. \tag{5.14}$$

If the condition

$$C_{\hat{\varrho}} := \sup_{\lambda\in\mathbb{R}}(1 + \lambda^2)\|\varrho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty \tag{5.15}$$

is satisfied, then

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \tag{5.16}$$
$$-i\operatorname{tr}(K\varrho(t)U(\omega)) + i\operatorname{tr}(\varrho(t)KU(\omega)) = -i\operatorname{tr}(K\varrho U(\omega)) + i\operatorname{tr}(\varrho KU(\omega)).$$

Hence

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \tag{5.17}$$
$$-i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \lambda\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) + i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \lambda\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)).$$

By formula (3.42) we find

$$\int_{\omega} dx\ \lambda(\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) = \tag{5.18}$$
$$\int_{\omega} dx\ \lambda \left\langle \varrho^t(\lambda) \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle.$$

Since $l(\psi^-(x,\lambda,\tau)) = \lambda\psi^-(x,\lambda,\tau)$ one gets

$$\int_{\omega} dx\ \lambda(\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) = \tag{5.19}$$
$$\int_{\omega} dx\ \left\langle \varrho^t(\lambda) \begin{pmatrix} l(\psi^-(x,\lambda,b)) \\ l(\psi^-(x,\lambda,a)) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle.$$

Hence

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \tag{5.20}$$
$$-i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \left\langle \varrho^t(\lambda) \begin{pmatrix} l(\psi^-(x,\lambda,b)) \\ l(\psi^-(x,\lambda,a)) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle +$$
$$i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \left\langle \varrho^t(\lambda) \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} l(\psi^-(x,\lambda,b)) \\ l(\psi^-(x,\lambda,a)) \end{pmatrix} \right\rangle$$

Let $\omega = [c,d] \subseteq [a,b]$. Integrating by parts and taking into account formula (4.7) we get

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \int_{\mathbb{R}} d\lambda\ \left\{ j_{\hat{\varrho}}(c,\lambda) - j_{\hat{\varrho}}(d,\lambda) \right\}. \tag{5.21}$$

The total current $j_{\hat{\varrho}}(x)$ at the point $x \in [a,b]$ is defined by

$$j_{\hat{\varrho}}(x) := \int_{\mathbb{R}} d\lambda\ j_{\hat{\varrho}}(x,\lambda). \tag{5.22}$$

This yields This yields

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = j_{\hat{\varrho}}(c) - j_{\hat{\varrho}}(d) \tag{5.23}$$

which shows that the change of the number of carriers in the set $[c,d]$ is equal to the difference between the incoming current $j_{\hat{\varrho}}(c)$ at point c and the outgoing current $j_{\hat{\varrho}}(d)$ at point d which very well corresponds to the physical intuition. Since by Proposition 4.1 the current density $j_{\hat{\varrho}}(x,\lambda)$ does not depend on $x \in [a,b]$ one gets

$j_{\hat{\varrho}}(d) = j_{\hat{\varrho}}(c)$ which again verifies (5.14). The relation (5.23) is the integral form of the so-called continuity equation which has the differential form

$$\frac{\partial}{\partial t} u_{\hat{\varrho}(t)}(x) + \frac{\partial}{\partial x} j_{\hat{\varrho}(t)}(x) = 0, \quad t \in \mathbb{R}, \quad x \in \Omega, \tag{5.24}$$

where $u_{\hat{\varrho}(t)}(x)$ is the carrier density at time $t \in \mathbb{R}$ and $j_{\varrho(t)}(x)$ is current density at time t given by (5.22). Since $u_{\hat{\varrho}(t)}(x) = u_{\hat{\varrho}}(x)$ is independent of t and $j_{\varrho(t)}(x)$ is independent of x the continuity equation (5.24) obviously holds in the present situation.

4. On the basis of the considerations above we are able to give a mathematically rigourous foundation of dissipative Schrödinger-Poisson systems. To this end we consider different species $\pm$ of particles (holes and electrons) and assume that that for these species the effective masses $m_\pm$, external potentials $V_0^\pm$ and coefficients $\kappa_a^\pm, \kappa_b^\pm \in \mathbb{C}_+$ are given. For each species this leads to different dissipative Schrödinger operators $H^\pm(V_\pm)$ defined in accordance with (1.12), (2.1) and (2.2). The potential V entering into the definition of the Schrödinger operators is different for different species. It takes the form

$$V_\pm := V_0^\pm \pm \varphi(u). \tag{5.25}$$

where the electrostatic potential φ is a solution of the Poisson equation (1.1) with boundary condition (1.3). The carrier densities $u^\pm$ entering into Poisson's equation are obtained from the dissipative Schrödinger operators $H^\pm(V_\pm)$ in accordance with Section 3. To this end we assume that the families of matrices $\{\varrho_\pm(\lambda)\}_{\lambda\in\mathbb{R}}$, which obey

$$C_{\hat{\varrho}_\pm} := \sup_{\lambda\in\mathbb{R}} \sqrt{\lambda^2+1}\|\varrho_\pm(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty, \tag{5.26}$$

are given and we define the carrier densities $u^\pm(x) := u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x)$ in accordance with Section 3, i.e., if $D^\pm(V_\pm)(x)$ are the carrier density observables at $x \in \Omega$ and at energy $\lambda \in \mathbb{R}$, then the carrier densities are computed by

$$u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x) = \int_{\mathbb{R}} d\lambda\, u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x,\lambda), \quad x \in \Omega, \tag{5.27}$$

where

$$u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x,\lambda) = \mathrm{tr}_{\mathbb{C}^2}(\varrho_\pm(\lambda) D^\pm(V_\pm)(x,\lambda)), \quad x \in \Omega, \quad \lambda \in \mathbb{R}. \tag{5.28}$$

Moreover, if $\mathrm{tr}_{\mathbb{C}^2}(\varrho_\pm(\cdot)) \in L^1(\mathbb{R})$ is valid, then the current densities $j^\pm_{\hat{\varrho}_\pm}$,

$$j^\pm_{\hat{\varrho}_\pm} = \int_{\mathbb{R}} d\lambda\, j^\pm_{\hat{\varrho}_\pm}(V_\pm)(\lambda) \tag{5.29}$$

are also well-defined and finite, cf. Section 4. The so described system is called a dissipative Schrödinger-Poisson system. We note that the total number of carriers $N^\pm(V_\pm)$ is given by

$$N^\pm(V_\pm) = \int_\Omega dx\, u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x) \tag{5.30}$$

and is not fixed.

In a forthcoming paper [13] we show that under suitable conditions on $\epsilon(\cdot)$, $C(\cdot)$, $m_\pm(\cdot)$, $V_0^\pm(\cdot)$, $\kappa_b^\pm$, $\kappa_a^\pm$ and $\varrho_\pm$ this dissipative Schrödinger-Poisson system always admits a self-consistent solution.

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Density and current of a dissipative Schrödinger operator

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Abstract

A net current flow through an open 1-dimensional Schrödinger-Poisson system is modeled by replacing self-adjoint boundary conditions by dissipative ones. To give a rigorous definition of carrier and current densities the well-known dilation theory of dissipative operators is used where the self-adjoint dilation is regarded as the Hamiltonian of a larger closed system which contains the open one. The carrier density turns out to be performed by the generalized eigenstates of the dilation while the current density is related to the characteristic function of the dissipative operator. A rigorous setup of a dissipative Schrödinger-Poisson system is outlined.

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Keywords

open Schrödinger-Poisson system, carrier and current density, dissipative Schrödinger operator, self-adjoint dilation, generalized eigenfunctions, characteristic function, density matrix

Contents

1 Introduction

Schrödinger-Poisson systems are of great interest in semiconductor physics. In the following we are interested in a Schrödinger-Poisson system on the interval $\Omega = [a, b]$ on the real axis $\mathbb{R}$. Systems of this type were considered in [9]. By φ we denote the electrostatic potential on Ω which is determined by Poisson's equation

$$-\frac{d}{dx}\epsilon(x)\frac{d}{dx}\varphi = q\left(C(x) + u^+ - u^-\right), \quad x \in \Omega, \tag{1.1}$$

where u^+ and u^- are the densities of holes and electrons, q is the magnitude of the elementary charge, $C(\cdot)$ is the so-called doping profile of the semiconductor devices and $\epsilon = \epsilon(x) > 0$ denotes the dielectric permittivity which satisfies the condition

$$\epsilon(\cdot) + \frac{1}{\epsilon(\cdot)} \in L^\infty([a, b]). \tag{1.2}$$

The Poisson equation (1.1) is completed by the boundary conditions

$$\varphi(a) = \varphi_a, \quad \text{and} \quad \varphi(b) = \varphi_b. \tag{1.3}$$

The second important ingredient of the Schrödinger-Poisson system are Schrödinger-type operators H which are defined on the Hilbert space $\mathfrak{H} = L^2([a, b])$ and look like

$$H := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx} + V, \tag{1.4}$$

where the real potential V is slightly different for holes and electrons, see Section 5, and m equals either to the x-dependent effective mass of the holes or of the electrons. Since the formalism of quantum mechanics is well developed only for self-adjoint operators usually self-adjoint boundary conditions, for instance Neuman or Dirichlet boundary conditions at a and b, are chosen. Operators of this type have a discrete spectrum. Let us denote by $\{\mathcal{E}_l\}_{l=1}^\infty$ and $\{\psi_l\}_{l=1}^\infty$ the sequence of eigenvalues and eigenfunctions counting multiplicities.

The carrier densities used in the Poisson equation are now performed by expressions of the form

$$u_{\hat{\varrho}}(x) = \sum_{l=1}^\infty \varrho_l |\psi_l(x)|^2, \quad x \in [a, b], \tag{1.5}$$

where $\hat{\varrho} := \{\varrho_l\}_{l=1}^\infty$ is a sequence of occupation numbers such that

$$N := \sum_{l=1}^\infty \varrho_l, \tag{1.6}$$

is the total number of carriers of the system. Usually, the sequence $\hat{\varrho}$ is given by

$$\varrho_l := f(\mathcal{E}_l), \quad l = 1, 2, \ldots . \tag{1.7}$$

where $f \geq 0$ is a equilibrium distribution functions which may be different for holes and electrons. Let us introduce the operator

$$\varrho := f(H). \tag{1.8}$$

The operator ϱ is self-adjoint and non-negative. If the equilibrium distribution function f tends to zero sufficiently fast as $x \to +\infty$, then ϱ is nuclear. From ϱ one computes the total number N of carriers by $N = \mathrm{tr}(\varrho) = \mathrm{tr}(f(H))$. Usually, non-negative self-adjoint nuclear operators are called density matrices. Since ϱ commutes with H the density matrix ϱ remains unchanged in time. In this case ϱ is called a steady state. If the density matrix is known, then one restores the carrier density as follows: the number of carriers $N_\varrho(\omega)$ in the set $\omega \subseteq [a,b]$ is computed by

$$N_\varrho(\omega) = \mathrm{tr}(\varrho\chi_\omega), \tag{1.9}$$

where $\chi_\omega(\cdot)$ is the indicator function of the subset ω. It turns out that (1.9) defines an absolutely continuous measure (with respect to the Lebesgue measure). One verifies that its Radon-Nikodym derivative u_ϱ coincides with the carrier density defined by (1.5), i.e. $u_{\hat{\varrho}} = u_\varrho$.

The system described by H is closed. Hence there is no interaction with the environment, in particular, no carrier exchange. Consequently, the current density $j_{\hat{\varrho}}(x)$ defined by

$$j_{\hat{\varrho}}(x) := \sum_{l=1}^{\infty} \varrho_l j_l(x), \quad x \in [a,b], \tag{1.10}$$

is identical zero, where in accordance with [15] the current density $j_l(x)$ of the eigenstate ψ_l is given by

$$j_l(x) := \Im\mathrm{m}\left(\frac{1}{m(x)}\psi_l'(x)\overline{\psi_l(x)}\right), \; x \in [a,b], \; l = 1,2,\ldots. \tag{1.11}$$

However, from the point of view of semiconductor physics this consequence is totally unacceptable since a net current flow through the boundary is natural. Thus one has to devise boundary conditions which allow those flows.

A simple proposal was made in [9] which adds up to replace the self-adjoint boundary conditions by non-selfadjoint ones, i.e. to consider H on the domain

$$\mathrm{dom}(H) = \left\{ g \in W^{1,2}([a,b]) : \begin{array}{l} \frac{1}{m(x)}g'(x) \in W^{1,2}([a,b]), \\ \frac{1}{2m(a)}g'(a) = -\kappa_a g(a), \\ \frac{1}{2m(b)}g'(b) = \kappa_b g(b) \end{array} \right\} \tag{1.12}$$

where $\kappa_a, \kappa_b \in \mathbb{C}$. If at least one of the imaginary parts is different from zero, then the operator H is non-selfadjoint. However, this non-selfadjointness implies several complications. In particular, the notion of carrier densities becomes unclear.

This situation can be handled if we restrict ourselves to dissipative operators. Let us recall that an operator is called dissipative if the imaginary part of its associated quadratic form is non-positive. In the present case the operator H is dissipative if $\kappa_a, \kappa_b \in \mathbb{C}_+ := \{z \in \mathbb{C} : \Im m(z) > 0\}$, see [11]. Moreover, under this assumption the operator H becomes maximal dissipative, i.e. it admits no proper dissipative extension, see [11]. The main technical tool to overcome the difficulties is the dilation theory for maximal dissipative operator. In [12] the minimal self-adjoint dilation K of H was explicitly constructed and analysed in detail. From the physical point of view the minimal self-adjoint dilation plays the role of the Hamiltonian of a larger closed system which contains the original system described by H. Using this fact one defines steady states, carrier densities and current densities. It turns out that the current density is independent of $x \in [a,b]$ and, in general, different from zero. So we have a constant current through $[a,b]$ which is quite satisfactory from the physical point of view.

It turns out that this formal approach to the net current flow problem fits into models discussed in the literature. Indeed, a well adopted model in semiconductor physics is the so-called Kirkner-Lent model [14] which was mathematically analysed in [4], [5] and [6]. In this model one replaces the maximal dissipative operator H by a family of maximal dissipative operators $\{H(z)\}_{z\in\overline{\mathbb{C}_+}}$ defined on $\mathfrak{H} = L^2([a,b])$ and given by

$$\begin{aligned} \mathrm{dom}(H(z)) &:= \left\{ g \in W^{2,2}([0,1]) : \begin{array}{l} g'(1) = \kappa_1(z)g(1) \\ g'(0) = -\kappa_0(z)g(0), \end{array} \right\}, \\ (H(z)g)(x) &:= -\tfrac{d^2}{dx^2}g(x) + V(x)g(x), \quad g \in \mathrm{dom}(H(z)), \end{aligned} \tag{1.13}$$

$m(x) \equiv 1/2$, with

$$\kappa_1(z) := i\sqrt{z} \quad \text{and} \quad \kappa_0(z) := i\sqrt{z - V_-}, \quad z \in \overline{\mathbb{C}_+}, \tag{1.14}$$

where the cut of the square root is along $[0,\infty)$ and $\Im m(\sqrt{z}) \geq 0$ for $z \in \mathbb{C}_+$. Let us consider the self-adjoint Schrödinger operator K,

$$\begin{aligned} \mathrm{dom}(K) &:= W^{2,2}(\mathbb{R}), \\ (Kf)(x) &:= -\tfrac{d^2}{dx^2}f(x) + V_{KL}(x)f(x), \quad f \in \mathrm{dom}(K), \end{aligned} \tag{1.15}$$

on the Hilbert space $\mathfrak{K} = L^2(\mathbb{R})$ whose potential $V_{KL} \in C(\mathbb{R})$ looks like

$$V_{KL} = \begin{cases} V_- & : \; x \in \mathbb{R}_- \\ V & : \; x \in [0,1] \\ 0 & : \; x \in (1,+\infty) \end{cases} \tag{1.16}$$

where $V_- > 0$,

$$V(0) = V_- \quad \text{and} \quad V(1) = 0. \tag{1.17}$$

Operators of this type were investigate in [7]. It turns out that

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K - z)^{-1}|\mathfrak{H} = (H(z) - z)^{-1}, \quad z \in \mathbb{C}_+. \tag{1.18}$$

which means that the operator K can be regarded as a self-adjoint dilation of the family $\{H(z)\}_{z\in\overline{\mathbb{C}_+}}$. Moreover, it holds

$$\bigvee_{z\in\mathbb{C}\setminus\mathbb{R}} (K-z)^{-1}\mathfrak{H} = \mathfrak{K} \tag{1.19}$$

which means that K is a minimal self-adjoint dilation and, hence, that K is unique up to a certain isomorphism. Thus, if we want to compute quantities which are related to the subspace $\mathfrak{H}$, for instance, carrier densities on the interval $[0,1]$, we can do this using either the self-adjoint operator K or the family $\{H(\lambda)\}_{\lambda\in\mathbb{R}}$ of maximal dissipative operators. Moreover, if we are only interested in quantities with respect to a small energy interval around the energy $\lambda_0 \in \mathbb{R}$ (in the limit only quantities for the energy λ_0), then it is enough to consider the maximal dissipative operator $H(\lambda_0)$ which leads to a model described at the beginning.

The paper is organized as follows. In Section 2 we rigorously define Schrödinger-type operators and briefly recall their properties, cf. [11]. Moreover, we introduce the important notion of the characteristic function $\Theta_H(z)$ and briefly describe the minimal self-adjoint dilation K of H. For further purposes we indicate its generalized eigenfunction expansion. Essentially, we follow here the paper [12]. In Section 3 we introduce generalized steady states and define carrier densities. In Section 4 we define the current density and compute it in terms of the characteristic function. In particular, it turns out that if the steady state is given by $\varrho = f(K)$, then the current density is zero. In Section 5 we comment the results, in particular, we clarify the relation to the Lax-Phillips scattering theory and verify the continuity equation. Finally, we give a rigorous setting of so-called dissipative Schrödinger-Poisson systems which have the advantage that their current densities are different from zero for suitable chosen steady states.

2 Schrödinger-type operators

Following the proposal of [9] we consider the non-selfadjoint Schrödinger-type operator H on the Hilbert space $\mathfrak{H} = L^2([a,b])$ given by the domain (1.12) and

$$(Hg)(x) = (l(g))(x), \quad g \in \mathrm{dom}(H), \tag{2.1}$$

where

$$(l(g))(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}g(x) + V(x)g(x), \tag{2.2}$$

and $V \in L^2([a,b])$ is a real potential, the effective mass $m(x) > 0$ obeys $m(x)+\frac{1}{m(x)} \in L^\infty([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. The operator H is maximal dissipative and completely non-selfadjoint, see [11]. The spectrum of H consists of isolated eigenvalues in the lower half-plane with the only accumulation point at infinity. Since the operator H is completely non-selfadjoint there do not exist real eigenvalues. To analyze the operator H it is useful to introduce the elementary solutions $v_a(x,z)$ and $v_b(x,z)$,

$$l(v_a(x,z)) - zv_a(x,z) = 0, \quad v_a(a,z) = 1, \quad \frac{1}{2m(a)}v_a'(a,z) = -\kappa_a, \tag{2.3}$$

$$l(v_b(x,z)) - zv_b(x,z) = 0, \quad v_b(b,z) = 1, \quad \frac{1}{2m(b)}v_b'(b,z) = \kappa_b, \tag{2.4}$$

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

$$W(z) = v_a(x,z)\frac{1}{2m(x)}v_b'(x,z) - v_b(x,z)\frac{1}{2m(x)}v_a'(x,z). \tag{2.5}$$

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

$$v_{*a}(x,z) := \overline{v_a(x,\overline{z})} \quad \text{and} \quad v_{*b}(x,z) := \overline{v_b(x,\overline{z})}, \quad z \in \mathbb{C}, \tag{2.6}$$

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

$$l(v_{*a}(x,z)) - zv_{*a}(x,z) = 0, \quad v_{*a}(a,z) = 1, \quad \frac{1}{2m(a)}v_{*a}'(a,z) = -\overline{\kappa_a}, \tag{2.7}$$

$$l(v_{*b}(x,z)) - zv_{*b}(x,z) = 0, \quad v_{*b}(b,z) = 1, \quad \frac{1}{2m(b)}v_{*b}'(b,z) = \overline{\kappa_b}, \tag{2.8}$$

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

$$\begin{aligned}&((H-z)^{-1}f)(x) = \\ &\qquad -\frac{v_b(x,z)}{W(z)}\int_a^x dy\, v_a(y,z)f(y) - \frac{v_a(x,z)}{W(z)}\int_x^b dy\, v_b(y,z)f(y),\end{aligned} \tag{2.9}$$

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

$$\begin{aligned}&((H^*-z)^{-1}f)(x) = \\ &\qquad -\frac{v_{*b}(x,z)}{W_*(z)}\int_a^x dy\, v_{*a}(y,z)f(y) - \frac{v_{*a}(x,z)}{W_*(z)}\int_x^b dy\, v_{*b}(y,z)f(y),\end{aligned} \tag{2.10}$$

for $z \in \varrho(H^*)$ and $f \in L^2([a,b])$, see [12].

Since H is completely non-selfadjoint the maximal dissipative operator H can be completely characterized by its characteristic function $\Theta_H(z)$, $z \in \varrho(H) \cap \varrho(H^*)$, cf. [8]. The definition of the characteristic function relies on the so-called boundary operators $T(z) : \mathfrak{H} \longrightarrow \mathbb{C}^2$, $z \in \varrho(H)$ and $T_*(z) : \mathfrak{H} \longrightarrow \mathbb{C}^2$, $z \in \varrho(H^*)$, which are defined in [12]. Writing

$$\kappa_a = q_a + \frac{i}{2}\alpha_a^2 \quad \text{and} \quad \kappa_b = q_b + \frac{i}{2}\alpha_b^2, \quad \alpha_a, \alpha_b > 0, \tag{2.11}$$

the boundary operators are defined by

$$T(z)f := \begin{pmatrix} \alpha_b((H-z)^{-1}f)(b) \\ -\alpha_a((H-z)^{-1}f)(a) \end{pmatrix} \tag{2.12}$$

and

$$T_*(z)f := \begin{pmatrix} \alpha_b((H^*-z)^{-1}f)(b) \\ -\alpha_a((H^*-z)^{-1}f)(a) \end{pmatrix}, \tag{2.13}$$

$f \in L^2([a,b])$. Using the resolvent representations (2.9) and (2.10) we obtain

$$T(z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\; v_a(y,z)f(y) \\ \alpha_a \int_a^b dy\; v_b(y,z)f(y) \end{pmatrix} \tag{2.14}$$

and

$$T_*(z)f = \frac{1}{W_*(z)} \begin{pmatrix} -\alpha_b \int_a^b dy\; v_{*a}(y,z)f(y) \\ \alpha_b \int_a^b dy\; v_{*b}(y,z)f(y) \end{pmatrix}, \tag{2.15}$$

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

$$\begin{aligned} \left(T(z)^*\xi\right)(x) &= \frac{1}{\overline{W(z)}} \left(-\alpha_b\overline{v_a(x,z)}, \alpha_a\overline{v_b(x,z)}\right)\xi \\ &= \frac{1}{W_*(\overline{z})} \left(-\alpha_b v_{*a}(x,\overline{z}), \alpha_a v_{*b}(x,\overline{z})\right)\xi, \end{aligned} \tag{2.16}$$

and

$$\begin{aligned} \left(T_*(z)^*\xi\right)(x) &= \frac{1}{\overline{W_*(z)}} \left(-\alpha_b\overline{v_{*a}(x,z)}, \alpha_a\overline{v_{*b}(x,z)}\right)\xi \\ &= \frac{1}{W(\overline{z})} \left(-\alpha_b v_a(x,\overline{z}), \alpha_a v_b(x,\overline{z})\right)\xi, \end{aligned} \tag{2.17}$$

where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^a \end{pmatrix} \in \mathbb{C}^2. \tag{2.18}$$

The characteristic function Θ_H of the maximal dissipative operator H is a two-by-two matrix-valued function which satisfies the relation

$$\Theta_H(z)T(z)f = T_*(z)f, \quad z \in \varrho(H)\cap\varrho(H^*), \tag{2.19}$$

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

$$\|\Theta_H(z)\| \le 1 \quad \text{for} \quad z \in \mathbb{C}_-. \tag{2.20}$$

Using the elementary solutions the characteristic function Θ_H takes the form

$$\Theta_H(z) = I_{\mathbb{C}^2} + i\frac{1}{W_*(z)} \begin{pmatrix} \alpha_b^2 v_{*a}(b,z) & -\alpha_b\alpha_a \\ -\alpha_b\alpha_a & \alpha_a^2 v_{*b}(a,z) \end{pmatrix}. \tag{2.21}$$

for $z \in \varrho(H) \cap \varrho(H^*)$, cf. [12]

Since H is a maximal dissipative operator there is a larger Hilbert space $\mathfrak{K} \supseteq \mathfrak{H}$ and a self-adjoint operator K on $\mathfrak{K}$ such that

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K - z)^{-1}|\mathfrak{H} = (H - z)^{-1}, \quad \Im\mathrm{m}(z) > 0, \tag{2.22}$$

see [8]. The operator K is called a self-adjoint dilation of the maximal dissipative operator H. Obviously, from the condition (2.22) one gets

$$P^{\mathfrak{K}}_{\mathfrak{H}}(K - z)^{-1}|\mathfrak{H} = (H^* - z)^{-1}, \quad \Im\mathrm{m}(z) < 0. \tag{2.23}$$

K is called a minimal self-adjoint dilation of H if the condition

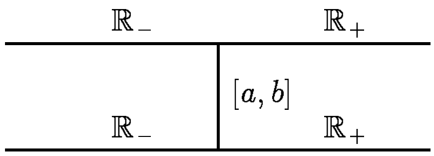
$$\bigvee_{z \in \mathbb{C}\setminus\mathbb{R}} (K - z)^{-1}\mathfrak{H} = \mathfrak{K} \tag{2.24}$$

is satisfied. 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. Following [12] we introduce the larger Hilbert space

$$\mathfrak{K} = \mathcal{D}_- \oplus \mathfrak{H} \oplus \mathcal{D}_+, \tag{2.25}$$

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



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

$$\vec{g} := g_- \oplus g \oplus g_+, \tag{2.26}$$

where

$$g_-(x) := \begin{pmatrix} g^b_-(x) \\ g^a_-(x) \end{pmatrix} \qquad \text{and} \quad g_+(x) := \begin{pmatrix} g^b_+(x) \\ g^a_+(x) \end{pmatrix}, \tag{2.27}$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively. Let the matrices $K^a_\pm$ and $K^b_\pm$ given by

$$K^a_- := \frac{1}{\alpha_a}\begin{pmatrix} 0 & 0 \\ 1 & \kappa_a \end{pmatrix} \qquad \text{and} \qquad K^a_+ := \frac{1}{\alpha_a}\begin{pmatrix} 0 & 0 \\ 1 & \overline{\kappa_a} \end{pmatrix} \tag{2.28}$$

as well as

$$K^b_- := \frac{1}{\alpha_b}\begin{pmatrix} 1 & -\kappa_b \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad K^b_+ := \frac{1}{\alpha_b}\begin{pmatrix} 1 & -\overline{\kappa_b} \\ 0 & 0 \end{pmatrix}. \tag{2.29}$$

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

$$\mathrm{dom}(K) := \left\{ \vec{g} \in \mathfrak{K} : \begin{array}{l} g_\pm \in W^{1,2}(\mathbb{R}_\pm, \mathbb{C}^2), \\ g, \frac{1}{m} g' \in W^{1,2}([a,b]), \\ K_-^a g_a + K_-^b g_b = g_-(0), \\ K_+^a g_a + K_+^b g_b = g_+(0) \end{array} \right\} \tag{2.30}$$

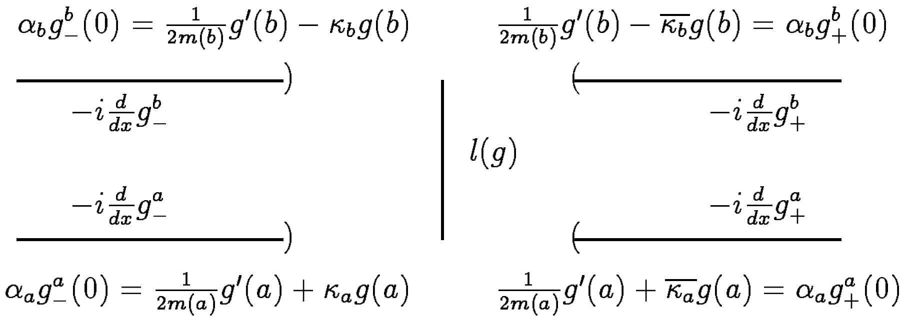
and

$$K\vec{g} := -i \frac{d}{dx} g_- \oplus l(g) \oplus -i \frac{d}{dx} g_+, \qquad \vec{g} \in \mathrm{dom}(K), \tag{2.31}$$

where

$$g_a = \begin{pmatrix} \frac{1}{2m(a)} g'(a) \\ g(a) \end{pmatrix} \quad \text{and} \quad g_b = \begin{pmatrix} \frac{1}{2m(b)} g'(b) \\ g(b) \end{pmatrix}. \tag{2.32}$$

With respect to a graph picture the operator K looks like



The self-adjoint operator K is absolutely continuous and its spectrum coincides with the real axis, i.e. $\sigma(K) = \mathbb{R}$. The multiplicity of its spectrum is two. The resolvent of K admits the representation

$$\begin{aligned} &(K - z)^{-1} (f_- \oplus f \oplus f_+) = \\ &i \int_{-\infty}^{x} dy\; e^{i(x-y)z} f_-(y) \;\oplus\; (H - z)^{-1} f + i T_*(\overline{z})^* \int_{-\infty}^{0} dy\; e^{-iyz} f_-(y) \;\oplus \\ &i \int_0^x dy\; e^{i(x-y)z} f_+(y) + i e^{izx} T(z) f + i \Theta_H(\overline{z})^* \int_{-\infty}^{0} dy\; e^{i(x-y)z} f_-(y) \end{aligned} \tag{2.33}$$

for $\Im\mathrm{m}(z) > 0$ and

$$\begin{aligned} &(K - z)^{-1} (f_- \oplus f \oplus f_+) = \\ &-i \int_x^0 dy\; e^{i(x-y)z} f_-(y) - i e^{izx} T_*(z) f - i \Theta_H(z) \int_0^\infty dy\; e^{i(x-y)z} f_+(y) \oplus \\ &(H^* - z)^{-1} f - i T(\overline{z})^* \int_0^\infty dy\; e^{-iyz} f_+(y) \;\oplus\; -i \int_x^\infty dy\; e^{i(x-y)z} f_+(y) \end{aligned} \tag{2.34}$$

for $\Im\mathrm{m}(z) < 0$. The generalized eigenfunctions $\vec{\psi}^-(\cdot, \lambda, \tau)$, $\lambda \in \mathbb{R}$, $\tau = a, b$, of K are given by

$$\begin{aligned} &\vec{\psi}^-(x, \lambda, \tau) := \psi_-^-(x, \lambda, \tau) \oplus \psi^-(x, \lambda, \tau) \oplus \psi_+^-(x, \lambda, \tau) = \\ &\frac{1}{\sqrt{2\pi}} e^{ix\lambda} e_\tau \oplus \frac{1}{\sqrt{2\pi}} (T_*(\lambda)^* e_\tau)(x) \oplus \frac{1}{\sqrt{2\pi}} e^{ix\lambda} \Theta_H(\lambda)^* e_\tau \end{aligned} \tag{2.35}$$

where

$$e_b := \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad e_a := \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.36}$$

The functions are mutually orthogonal, i.e. one has

$$\left(\vec{\psi}^-(\cdot,\lambda,\tau),\vec{\psi}^-(\cdot,\lambda',\tau')\right)_{L^2(\hat{\Omega})} = \delta(\lambda-\lambda')\delta_{\tau\tau'}, \tag{2.37}$$

in the sense of distribution for $\lambda,\lambda' \in \mathbb{R}$, $\tau,\tau' = a,b$. Moreover, elements of the form

$$\int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}^-(\cdot,\lambda,\tau)\hat{g}^\tau(\lambda) \tag{2.38}$$

where $\hat{g}^\tau(\cdot)$, $\tau = a,b$, are smooth functions with compact support, are dense in $\mathfrak{K}$. We note that the generalized eigenfunctions $\vec{\psi}^-(\cdot,\lambda,\tau)$ are usually called the incoming eigenfunctions. Using the incoming eigenfunctions one defines a transformation $\Phi_- : \mathfrak{K} \longrightarrow \hat{\mathfrak{K}} = L^2(\mathbb{R},\mathbb{C}^2)$

$$(\Phi_-\vec{g})(\lambda) =: \hat{g}(\lambda) = \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix}, \tag{2.39}$$

where

$$\hat{g}^\tau(\lambda) := \int_{\hat{\Omega}} dx \left(\vec{g}(x),\vec{\psi}^-(x,\lambda,\tau)\right), \quad \tau = a,b. \tag{2.40}$$

Φ_- is unitary and called the incoming Fourier transformation. The inverse incoming Fourier transformation Φ_-^{-1} is given by

$$(\Phi_-^{-1}\hat{g})(x) = \int_{\mathbb{R}} d\lambda \sum_{\tau=a,b} \vec{\psi}^-(x,\lambda,\tau)\hat{g}^\tau(\lambda), \quad \hat{g} \in L^2(\mathbb{R},\mathbb{C}^2). \tag{2.41}$$

We note that

$$\Phi_- K \Phi_-^{-1} = M \tag{2.42}$$

where M is the multiplication operator by the independent variable λ on $\hat{\mathfrak{K}}$, i.e.

$$\begin{aligned} \mathrm{dom}(M) &:= \left\{\hat{g} \in L^2(\mathbb{R},\mathbb{C}^2) : \lambda\hat{g}(\lambda) \in L^2(\mathbb{R},\mathbb{C}^2)\right\}, \\ (M\hat{g})(\lambda) &:= \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathrm{dom}(M). \end{aligned} \tag{2.43}$$

The representation (2.43) induced by Φ_- is called the incoming spectral representation of K.

Finally, we note that each bounded self-adjoint operator G on $\mathfrak{K}$, which commutes with K, corresponds to a measurable family $\{G(\lambda)\}_{\lambda\in\mathbb{R}}$ of two-by-two matrices, which are uniformly bounded, i.e., $G(\cdot) \in L^\infty(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$, such that the multiplication operator $\hat{G}$ on $L^2(\mathbb{R},\mathbb{C}^2)$ defined by

$$\begin{aligned} \mathrm{dom}(\hat{G}) &:= \left\{\hat{g} \in L^2(\mathbb{R},\mathbb{C}^2) : G(\lambda)\hat{g}(\lambda) \in L^2(\mathbb{R},\mathbb{C}^2)\right\}, \\ (\hat{G}\hat{g})(\lambda) &:= G(\lambda)\hat{g}(\lambda), \quad \hat{g} \in \mathrm{dom}(\hat{G(\cdot)}) \end{aligned} \tag{2.44}$$

is unitarily equivalent to G, i.e.

$$\Phi_- G \Phi_-^{-1} = \hat{G}. \tag{2.45}$$

Indeed, if G commutes with K, then $\hat{G}$ commutes with M. Applying Theorem VII.2.3 of [3] one immediately gets that $\hat{G}$ is a multiplication operator of type (2.44). The representation (2.44) is called the incoming spectral representation of G.

3 Carrier density

In the following we call an operator $\varrho : \mathfrak{K} \longrightarrow \mathfrak{K}$ a density matrix if ϱ is a bounded, non-negative operator. The operator ϱ is called a steady state if ϱ commutes with K. Obviously, a steady state does not change in time. If ϱ is a steady state, then there is a measurable matrix-valued function $\varrho(\cdot) \in L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that the multiplication operator $\hat{\varrho}$ on $L^2(\mathbb{R}, \mathbb{C}^2)$ generated by $\varrho(\cdot)$ is unitarily equivalent to ϱ, i.e.

$$\varrho = \Phi_-^{-1} \hat{\varrho} \Phi_-, \tag{3.1}$$

see above. Obviously, the measurable function $\varrho(\cdot)$ takes the form

$$\varrho(\lambda) = \begin{pmatrix} \varrho^{bb}(\lambda) & \varrho^{ba}(\lambda) \\ \varrho^{ab}(\lambda) & \varrho^{aa}(\lambda) \end{pmatrix} \tag{3.2}$$

where $\varrho^{\tau\nu}(\cdot) \in L^\infty(\mathbb{R})$, $\tau, \nu = a, b$. Since $\varrho \geq 0$ one gets that $\varrho(\lambda) \geq 0$ a.e. (with respect to the Lebesgue measure).

Definition 3.1 A bounded self-adjoint operator A on $\mathfrak{K}$ is called an observable. We say the observable A

(i) is admissible with respect to ϱ if ϱA is a nuclear operator on $\mathfrak{K}$, i.e. $\varrho A \in \mathcal{L}_1(\mathfrak{K})$,

(ii) is admissible with respect to K if $E_K(\Delta)A \in \mathcal{L}_1(\mathfrak{K})$ for each bounded interval $\Delta \subseteq \mathbb{R}$ where $E_K(\cdot)$ denotes the spectral measure of K.

If the observable A is admissible with respect to ϱ, then its expectation value $\mathbb{E}_\varrho(A)$ with respect to the density matrix ϱ is defined by

$$\mathbb{E}_\varrho(A) := \mathrm{tr}(\varrho A). \tag{3.3}$$

In the following we show that the admissibility of A with respect to K leads to a certain localization in the incoming spectral representation:

Proposition 3.2 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. If the observable A is admissible with respect to K, then there exists a measurable* *matrix-valued function $A(\cdot) \in L^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$, such that $A(\lambda) = A(\lambda)^*$ for a.e. $\lambda \in \mathbb{R}$ and*

$$\operatorname{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \, \operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda) A(\lambda)) \tag{3.4}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$ and any steady state ϱ of K. The measurable function $A(\cdot)$ is uniquely defined up to a Borel set of Lebesgue measure zero.

If the observable A is in addition admissible with respect to the steady state ϱ, then $\operatorname{tr}_{\mathbb{C}^2}(\varrho(\cdot)A(\cdot)) \in L^1(\mathbb{R})$ and the representation

$$\operatorname{tr}(\varrho A) = \int_{\mathbb{R}} d\lambda \, \operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda) A(\lambda)) \tag{3.5}$$

holds.

Proof. Notice that the spectral measure $E_K(\cdot)$ of K is absolutely continuous with respect to Lebesgue measure. Hence, the set function

$$\mu_{\varrho,A}(\Delta) := \operatorname{tr}(\varrho A E_K(\Delta)), \tag{3.6}$$

where Δ is bounded Borel set of $\mathbb{R}$, is in fact a Lebesgue absolutely continuous measure. Let $\frac{d\mu_{\varrho,A}}{d\lambda}$ denote its Radon-Nikodym derivative and define

$$T_A(\hat{\varrho}) := \frac{d\mu_{\varrho,A}}{d\lambda}. \tag{3.7}$$

Then $T_A(\cdot)$ maps $L^\infty(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ continuously into $L^1_{loc}(\mathbb{R})$ (the latter in its canonic Frechet topology) and, additionally, one has

$$\operatorname{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \, \frac{d\mu_{\varrho,A}}{d\lambda}(\lambda) = \int_\Delta d\lambda \, T_A(\hat{\varrho})(\lambda) \tag{3.8}$$

for any bounded Borel set $\Delta \subset \mathbb{R}$. It is not hard to see that (3.8) implies the equality

$$T_A(\chi_\Delta \hat{\varrho}) = \chi_\Delta T_A(\hat{\varrho}) \tag{3.9}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$ where χ_Δ denotes its indicator function. We put

$$e_{bb} := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \; e_{ba} := \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \; e_{ab} := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \; e_{aa} := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{3.10}$$

and define for any $h \in L^\infty(\mathbb{R})$

$$A_{ij}(h) := T_A(h \cdot e_{ji}), \qquad i, j = a, b. \tag{3.11}$$

Clearly, each of the mappings $A_{ij}(\cdot)$ then maps $L^\infty(\mathbb{R})$ continuously into $L^1_{loc}(\mathbb{R})$ and (3.11) implies

$$A_{ij}(\chi_\Delta h) = \chi_\Delta A_{ij}(h) \tag{3.12}$$

for any $h \in L^\infty(\mathbb{R})$ and any Borel set Δ. Taking in particular $h \equiv 1$, this yields

$$A_{ij}(\chi_\Delta) = \chi_\Delta A_{ij}(1). \tag{3.13}$$

Obviously, by the linearity of the mappings $A_{ij}(\cdot)$, this last equation remains true if χ_Δ is there replaced by any (finite) linear combination of indicator functions. Because the set of finite linear combinations of indicator functions is dense in $L^\infty(\mathbb{R})$, one gets for all $h \in L^\infty(\mathbb{R})$ the equation

$$A_{ij}(h) = h \cdot A_{ij}(1). \tag{3.14}$$

Since

$$\varrho(\cdot) = \varrho^{bb}(\cdot)e_{bb} + \varrho^{ba}(\cdot)e_{ba} + \varrho^{ab}(\cdot)e_{ab} + \varrho^{aa}(\cdot)e_{aa} \tag{3.15}$$

one gets

$$\begin{gathered}\operatorname{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda\; T_A(\hat{\varrho})(\lambda) = \\ \sum_{i,j=a,b} \int_\Delta d\lambda\; A_{ij}(\varrho^{ij})(\lambda) = \sum_{i,j=a,b} \int_\Delta d\lambda\; \varrho^{ij}(\lambda) A_{ji}(1)(\lambda).\end{gathered} \tag{3.16}$$

Setting

$$A(\cdot) := \begin{pmatrix} A_{bb}(1)(\cdot) & A_{ba}(1)(\cdot) \\ A_{ab}(1)(\cdot) & A_{aa}(1)(\cdot) \end{pmatrix} \tag{3.17}$$

we finally obtain (3.4) for any bounded Borel set $\Delta \subset \mathbb{R}$ and any steady state ϱ of K.

Assume that $\tilde{A}(\cdot)$ obeys also the conditions of the proposition. Setting $G(\lambda) := A(\lambda) - \tilde{A}(\lambda)$, $\lambda \in \mathbb{R}$, one gets that

$$\int_\Delta \operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda)G(\lambda)) = 0 \tag{3.18}$$

for any bounded Borel set Δ and any steady state ϱ. Hence $\operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda)G(\lambda)) = 0$ for a.e. λ and any steady state ϱ which immediately yields $G(\lambda) = 0$ or $A(\lambda) = \tilde{A}(\lambda)$ for a.e. $\lambda \in \mathbb{R}$.

If ϱ is admissible with respect to A, then $|\operatorname{tr}(\varrho A E_K(\Delta)| < \|\varrho A\|_{\mathcal{L}_1}$ for any Borel set $\Delta \subseteq \mathbb{R}$. By (3.4) this implies that $\operatorname{tr}(\varrho(\cdot)A(\cdot)) \in L^1(\mathbb{R})$. Since one has $\lim_{\Delta\uparrow\mathbb{R}} \operatorname{tr}(\varrho A E_K(\Delta)) = \operatorname{tr}(\varrho A)$ we obtain from (3.4) the equality (3.5). □

Proposition 3.2 says that the averaging procedure localizes with respect to the incoming spectral representation. Indeed, the quantity $\operatorname{tr}(\varrho(\lambda)A(\lambda))$ can be regarded as the local average of the observable $A(\lambda)$ with respect to the density matrix $\varrho(\lambda)$ at energy $\lambda \in \mathbb{R}$, i.e.

$$\mathbb{E}_{\varrho(\lambda)}(A(\lambda)) := \operatorname{tr}(\varrho(\lambda)A(\lambda)). \tag{3.19}$$

Formula (3.5) has the meaning that the total average $\mathbb{E}_\varrho(A)$ is the sum of the local averages $\mathbb{E}_{\varrho(\lambda)}(A(\lambda))$, i.e.

$$\mathbb{E}_\varrho(A) = \int_{\mathbb{R}} d\lambda\; \mathbb{E}_{\varrho(\lambda)}(A(\lambda)). \tag{3.20}$$

Proposition 3.2 gives rise to the following

Definition 3.3 Let A be an observable which is admissible with respect to K. An element $A(\cdot) \in L^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ is called a localizer of A with respect to K if $A(\lambda)^* = A(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ and

$$\operatorname{tr}(\varrho A E_K(\Delta)) = \int_\Delta d\lambda \ \operatorname{tr}(\varrho(\lambda)A(\lambda)) \tag{3.21}$$

holds for any bounded Borel subset $\Delta \subseteq \mathbb{R}$ and any steady state ϱ.

Proposition 3.2 says that an observable which is admissible with respect to K has always a unique localizer.

To calculate the carrier density we consider the observable $U(\omega)$, $\omega \subseteq \Omega$, given by

$$(U(\omega)\vec{f}\,)(x) = 0 \oplus \chi_\omega(x) f(x) \oplus 0, \quad \vec{f} \in L^2(\hat{\Omega}), \tag{3.22}$$

for any Borel subset $\omega \subseteq \Omega$. We note that the observable $U(\omega)$ is a projection on $\mathfrak{K}$ with $\operatorname{ran}(U(\omega)) \subseteq \mathfrak{H}$. Loosely speaking, the projection acts in fact only on the subspace $\mathfrak{H} \subseteq \mathfrak{K}$.

Lemma 3.4 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then for any Borel set $\omega \subseteq \Omega$ the observable $U(\omega)$ is admissible with respect to the minimal self-adjoint dilation K of the maximal dissipative operator H. If the steady state ϱ satisfies the condition*

$$C_{\hat{\varrho}} := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2 + 1}\,\|\varrho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty, \tag{3.23}$$

then for any Borel set $\omega \subseteq \Omega$ the observable $U(\omega)$ is admissible with respect to ϱ.

Proof. The relation (2.33) implies

$$U(\omega)(K-z)^{-1}\vec{f} = 0 \oplus \chi_\omega (H-z)^{-1} f + i\chi_\omega T_*(\overline{z})^* \int_{-\infty}^0 dy\ e^{-iyz} f_-(y) \ \oplus 0 \tag{3.24}$$

for $\vec{f} \in \mathfrak{K}$ and $z \in \mathbb{C}_+$. By Theorem 3.1 of [11] one gets that $(H-z)^{-1}$ is a trace class operator for each $z \in \mathbb{C}_+$. Hence $U(\omega)(H-z)^{-1}$ is a trace class operator for each $\omega \subseteq \Omega$. Since the operator $T_*(\overline{z})^*$ acts from the two dimensional Hilbert space $\mathbb{C}^2$ into $\mathfrak{H}$ one easily gets that the second addend of (3.24) is a trace class operator, too. Hence $U(\omega)(K-z)^{-1} \in \mathcal{L}_1(\mathfrak{K})$ for each Borel set $\omega \subseteq \Omega$ and $z \in \mathbb{C}_+$. Using the representation

$$U(\omega)E_K(\Delta) = U(\omega)(K-z)^{-1}(K-z)E_K(\Delta), \quad z \in \mathbb{C}_+, \tag{3.25}$$

we find that $U(\omega)E_K(\Delta)$ is a trace class operator for each Borel sets $\omega \subseteq \Omega$ and each bounded interval $\Delta \subseteq \mathbb{R}$. Hence, the observable $U(\omega)$ is admissible with respect to K for each Borel set $\omega \subseteq \Omega$.

Moreover, taking into account (3.23) and the representation

$$U(\omega)\,\varrho = U(\omega)(K-i)^{-1}(K-i)\varrho \tag{3.26}$$

one immediately gets that $U(\omega)\,\varrho$ is a trace class operator for each $\omega \subseteq \Omega$, because $(K-i)\varrho$ is bounded. Hence, $\varrho\, U(\omega)$ is a trace class operator for each Borel set $\omega \subseteq \Omega$ which yields that $U(\omega)\,\varrho$ is admissible with respect to ϱ □

Since $U(\omega)$ is admissible with respect to K for any Borel set $\omega \subseteq \Omega$ by Proposition 3.2 there is a unique localizer $U(\omega)(\cdot) : \mathbb{R} \longrightarrow \mathcal{B}(\mathbb{C}^2)$. We are going to calculate this localizer.

Proposition 3.5 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then for any Borel set $\omega \subseteq \Omega$ the localizer of $U(\omega)(\cdot)$ of the observable $U(\omega)$ is given by*

$$U(\omega)(\lambda) = \int_\omega dx\; D(x,\lambda) \tag{3.27}$$

where

$$D(x,\lambda) := \begin{pmatrix} |\psi^-(x,\lambda,b)|^2 & \psi^-(x,\lambda,a)\overline{\psi^-(x,\lambda,b)} \\ \psi^-(x,\lambda,b)\overline{\psi^-(x,\lambda,a)} & |\psi^-(x,\lambda,a)|^2 \end{pmatrix} \tag{3.28}$$

$x \in \Omega$, $\lambda \in \mathbb{R}$.

If the steady state ϱ satisfies the condition (3.23), then

$$\mathbb{E}_\varrho(U(\omega)) = \int_{\mathbb{R}} d\lambda\; \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\,U(\omega)(\lambda)) \tag{3.29}$$

for any Borel subset $\omega \subseteq \Omega$.

Proof. By Lemma 3.4 the observable $U(\omega)$ is admissible for any Borel set $\omega \subseteq \Omega$. By Proposition 3.2 there is a unique localizer $U(\omega)(\cdot) \in \mathcal{L}^1_{loc}(\mathbb{R}, \mathcal{B}(\mathbb{C}^2))$ such that (3.21) is satisfied for any bounded Borel set $\Delta \subseteq \mathbb{R}$ and any steady state ϱ. Following the proof of Proposition 3.2 we consider the measure

$$\mu_{\varrho,U(\omega)}(\Delta) = \mathrm{tr}(\varrho\, U(\omega) E_K(\Delta)) \tag{3.30}$$

for any bounded Borel set $\Delta \subseteq \mathbb{R}$. We set $\hat{U}(\omega) := \Phi_- U(\omega)\Phi_-^{-1}$ and $\hat{U}_\Delta(\omega) := E_M(\Delta)\hat{U}E_M(\Delta)$ where $M = \Phi_- K \Phi_-^{-1}$, see (2.42). By Lemma 3.4 the operator $\hat{U}_\Delta(\omega)$ is nuclear. Hence, we find

$$\mu_{\varrho,U(\omega)}(\Delta) = \mathrm{tr}(\hat{\varrho}\;\hat{U}_\Delta(\omega)). \tag{3.31}$$

Let us calculate the kernel of $\hat{U}_\Delta(\omega)$. To his end we consider the scalar product $(\hat{U}_\Delta(\omega)\hat{g}, \hat{f})$, $\hat{g}, \hat{f} \in L^2(\Delta, \mathbb{C}^2)$. Using (2.41) one has

$$(\hat{U}_\Delta(\omega)\hat{g}, \hat{f}) = \tag{3.32}$$
$$\int_\omega dx \int_\Delta d\lambda \sum_{\tau=a,b} \psi^-(x,\lambda,\tau)\hat{g}^\tau(\lambda)\overline{\int_\Delta d\mu \sum_{\xi=a,b} \psi^-(x,\mu,\xi)\hat{f}^\xi(\mu)}.$$

Setting

$$U_\Delta^{\tau\xi}(\omega)(\mu,\lambda) := \int_\omega dx\, \psi^-(x,\lambda,\xi)\overline{\psi^-(x,\mu,\tau)}, \quad \tau,\xi = a,b, \tag{3.33}$$

we get

$$(\hat{U}_\Delta(\omega)\hat{g},\hat{f}) = \tag{3.34}$$
$$\int_\Delta d\mu \left(\int_\Delta d\lambda \begin{pmatrix} U_\Delta^{bb}(\omega)(\mu,\lambda) & U_\Delta^{ba}(\omega)(\mu,\lambda) \\ U_\Delta^{ab}(\omega)(\mu,\lambda) & U_\Delta^{aa}(\omega)(\mu,\lambda) \end{pmatrix} \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix}, \begin{pmatrix} \hat{f}^b(\mu) \\ \hat{f}^a(\mu) \end{pmatrix}\right)$$

what shows that

$$U_\Delta(\omega)(\mu,\lambda) := \begin{pmatrix} U_\Delta^{bb}(\omega)(\mu,\lambda) & U_\Delta^{ba}(\omega)(\mu,\lambda) \\ U_\Delta^{ab}(\omega)(\mu,\lambda) & U_\Delta^{aa}(\omega)(\mu,\lambda) \end{pmatrix} \tag{3.35}$$

is the kernel of the integral operator $\hat{U}_\Delta(\omega)$. Setting

$$D(x,\mu,\lambda) := \begin{pmatrix} \psi^-(x,\lambda,b)\overline{\psi^-(x,\mu,b)} & \psi^-(x,\lambda,a)\overline{\psi^-(x,\mu,b)} \\ \psi^-(x,\lambda,b)\overline{\psi^-(x,\mu,a)} & \psi^-(x,\lambda,a)\overline{\psi^-(x,\mu,a)} \end{pmatrix} \tag{3.36}$$

we obtain the representation

$$U_\Delta(\omega)(\mu,\lambda) = \int_\omega dx\; D(x,\mu,\lambda),\;\; \mu,\lambda\in\Delta. \tag{3.37}$$

Since $U_\Delta(\omega)(\mu,\lambda) = U_{\Delta'}(\omega)(\mu,\lambda)$ for $\mu,\lambda \in \Delta \subseteq \Delta'$ it makes sense to define $U(\omega)(\mu,\lambda) := \lim_{\Delta\uparrow\mathbb{R}} U_\Delta(\omega)(\mu,\lambda)$, $\mu,\lambda\in\mathbb{R}$. Hence $U_\Delta(\omega)(\mu,\lambda) = U(\omega)(\mu,\lambda)$ for $\mu,\lambda\in\Delta$ and

$$U(\omega)(\mu,\lambda) = \int_\omega dx\; D(x,\mu,\lambda), \quad \mu,\lambda\in\Delta. \tag{3.38}$$

Since the kernel depends continuously on μ and λ one gets that

$$\operatorname{tr}(\hat{\varrho}\,\hat{U}_\Delta(\omega)) = \int_\Delta d\lambda\; \operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda)\; U(\omega)(\lambda,\lambda)) \tag{3.39}$$

for any bounded Borel set $\Delta\subseteq\mathbb{R}$ and any steady state ϱ. From (3.38) we find that $U(\omega)(\lambda,\lambda)^* = U(\omega)(\lambda,\lambda)$ for $\lambda\in\mathbb{R}$. Since the eigenfunctions $\psi^-(x,\lambda,b)$ and $\psi^-(x,\lambda,a)$ are bounded on compact sets of x and λ we obtain that $U(\omega)(\lambda,\lambda) \in L^1_{loc}(\mathbb{R},\mathcal{B}(\mathbb{C}^2))$. By (3.39) the matrix-valued function $U(\omega)(\lambda) := U(\omega)(\lambda,\lambda)$, $\lambda\in\mathbb{R}$, is the unique localizer of the observable $U(\omega)$. By condition (3.23) the observable $U(\omega)$ is admissible with respect to ϱ. Applying Proposition 3.2 we verify (3.29).

It remains to verify (3.27) and (3.28). From (3.38) and (3.39) we obtain the representation

$$\operatorname{tr}(\hat{\varrho}\,\hat{U}_\Delta(\omega)) = \int_\Delta d\lambda \int_\omega dx\; \operatorname{tr}_{\mathbb{C}^2}(\varrho(\lambda)\; D(x,\lambda,\lambda)). \tag{3.40}$$

Setting $D(x,\lambda) := D(x,\lambda,\lambda)$, $x\in\Omega$. $\lambda\in\mathbb{R}$, we immediately obtain (3.27) and (3.28). □

We set

$$u_{\hat{\varrho}}(x,\lambda) := \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\ D(x,\lambda)) \tag{3.41}$$

for $x \in \Omega$ and $\lambda \in \mathbb{R}$. A simple computation shows that the eigenvalues of $D(x,\lambda)$ are equal to $|\psi^-(x,\lambda,b)|^2$ and $|\psi^-(x,\lambda,a)|^2$ which shows that the matrix $D(x,\lambda)$ is non-negative for each $x \in \Omega$ and $\lambda \in \mathbb{R}$. Since for a.e. $\lambda \in \mathbb{R}$ the matrix $\varrho(\lambda)$ is non-negative, too one gets that $u_{\hat{\varrho}}(x,\lambda) \geq 0$ for $x \in \Omega$ and a.e. $\lambda \in \mathbb{R}$. This fact can also be verified taking into account the representation

$$u_{\hat{\varrho}}(x,\lambda) = \left\langle \varrho^t(\lambda) \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle \tag{3.42}$$

where $\varrho^t(\lambda)$ is the transposed matrix to (3.2). Moreover, if condition (3.23) is satisfied, then from Proposition (3.5) we obtain the representation

$$\mathbb{E}_\varrho(U(\omega)) = \int_{\mathbb{R}} d\lambda \int_\omega dx\ u_{\hat{\varrho}}(x,\lambda) \tag{3.43}$$

for Borel sets $\omega \subseteq \Omega$. Taking into account Fubini's theorem we find that

$$\mathbb{E}_\varrho(U(\omega)) = \int_\omega dx\ u_{\hat{\varrho}}(x). \tag{3.44}$$

where

$$u_{\hat{\varrho}}(x) := \int_{\mathbb{R}} d\lambda\ u_{\hat{\varrho}}(x,\lambda) \geq 0, \quad x \in \Omega, \tag{3.45}$$

and $u_{\hat{\varrho}} \in L^1(\Omega)$. The representation (3.44) shows that $\mathbb{E}_\varrho(U(\cdot))$ defines a measure on Ω which is absolutely continuous with respect to the Lebesgue measure. Since the expectation value $\mathbb{E}_\varrho(U(\omega))$ has the meaning of the number of carriers in $\omega \subseteq \Omega$ its Radon-Nikodym derivative can be interpreted as the carrier density of the system described by K and mutatis mutandis by H.

Definition 3.6 Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then the matrix $D(x,\lambda)$, $x \in \Omega$, and the value $u_{\hat{\varrho}}(x,\lambda)$ are called carrier density observable and carrier density at $x \in \Omega$ and at energy $\lambda \in \mathbb{R}$ of the system described by H, respectively.

This definition is justified by the fact that by (3.41) the carrier density $u_{\hat{\varrho}}(x,\lambda)$ is the expectation value of the carrier density observable $D(x,\lambda)$, i.e. $u_{\hat{\varrho}}(x,\lambda) = \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda))$ at $x \in \Omega$ and at $\lambda \in \mathbb{R}$. Moreover, we note that (3.45) can be written as

$$u_{\hat{\varrho}}(x) = \int_{\mathbb{R}} d\lambda\ \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)), \quad x \in \Omega, \tag{3.46}$$

i.e, the carrier density at $x \in \Omega$ is the sum of expectation values of the carrier density observable at $x \in \Omega$ over all energies.

On the Hilbert space $\mathfrak{K} = L^2(\hat{\Omega})$ we consider the multiplication operator $M(h)$,

$$(M(h)\vec{f})(x) = 0 \oplus h(x)f(x) \oplus 0, \quad x \in \Omega, \tag{3.47}$$

for real functions $h \in L^\infty(\Omega)$. We note that $M(\chi_\omega) = U(\omega)$ for any Borel set $\omega \subseteq \Omega$. In particular, one has $M(\chi_\Omega) = U(\Omega) = P_{\mathfrak{H}}^{\mathfrak{K}}$. Obviously, the representation

$$\varrho\, M(h) = \varrho\, U(\Omega)\, M(h), \quad h \in L^\infty(\Omega), \tag{3.48}$$

is valid. Since the observable $U(\Omega)$ is admissible with respect to ϱ the product $\varrho\, U(\Omega)$ is a nuclear operator on $\mathfrak{K}$ which yields that $\varrho M(h)$ is a nuclear operator on $\mathfrak{K}$, i.e. the observable $M(h)$ is admissible with respect to ϱ.

Proposition 3.7 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. If the steady state ϱ satisfies the condition (3.23), then the carrier density $u_{\hat{\varrho}}$ defined by (3.45) is a non-negative L^1-function such that*

$$\operatorname{tr}(\varrho M(h)) = \int_\Omega dx\; u_{\hat{\varrho}}(x) h(x) \tag{3.49}$$

for real functions $h \in L^\infty(\Omega)$. In particular, one has

$$\|u_{\hat{\varrho}}\|_{L^1(\omega)} = \operatorname{tr}(\varrho\, U(\omega)) \le C_{\hat{\varrho}} \|(K-i)^{-1} P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathcal{L}_1(\mathfrak{K})} \tag{3.50}$$

for each Borel set $\omega \subseteq \Omega$.

Proof. Setting $\omega = \Omega$ we obtain from (3.44) that $u_{\hat{\varrho}} \in L^1(\Omega)$. We choose $h = \chi_\omega$, $\omega \subseteq \Omega$. By (3.44) we get

$$\operatorname{tr}(\varrho M(\chi_\omega)) = \int_\Omega dx\; u_{\hat{\varrho}}(x) \chi_\omega(x). \tag{3.51}$$

By linearity this equation extends to

$$\operatorname{tr}(\varrho M(h)) = \int_\Omega dx\; u_{\hat{\varrho}}(x) h(x) \tag{3.52}$$

where h is an arbitrary step function on Ω. Since $u_{\hat{\varrho}}$ is from $L^1(\Omega)$ and $\varrho U(\Omega)$ is a nuclear operator both sides of (3.52) admit a continuation to L^∞-functions which verifies (3.49).

It remains to show the estimate (3.50). From (3.44) we immediately get

$$\int_\Omega dx\; u_g(x) = \operatorname{tr}(\varrho U(\Omega)) = \operatorname{tr}(\varrho (K-i)(K-i)^{-1} U(\Omega)). \tag{3.53}$$

Since $U(\Omega)(K-i)^{-1} \in \mathcal{L}_1(\mathfrak{K})$ and $\varrho(K-i)$ is a bounded operator which norm can be estimated by $C_{\hat{\varrho}}$ we obtain

$$\operatorname{tr}(\varrho (K-i)(K-i)^{-1} U(\omega)) \le C_{\hat{\varrho}} \|(K-i)^{-1} P_{\mathfrak{H}}^{\mathfrak{K}}\|_{\mathcal{L}_1(\mathfrak{K})} \tag{3.54}$$

which verifies (3.50). $\square$

Obviously, the relation (3.49) takes the form

$$\operatorname{tr}(\varrho M(h)) = \langle u_{\hat{\varrho}}, h\rangle_{L^1} \tag{3.55}$$

where by $\langle \cdot, h\rangle_{L^1}$, $h \in L^\infty(\Omega)$, we denote the linear functionals on $L^1(\Omega)$.

We conclude this section with some considerations which we need in the following section. Since $\{\varrho(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of non-negative self-adjoint operators there is a measurable family $\{V(\lambda)\}_{\lambda\in\mathbb{R}}$ of unitary operators on $\mathbb{C}^2$ such that

$$\varrho(\lambda) = V(\lambda)\begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V(\lambda)^* \tag{3.56}$$

for a.e. $\lambda \in \mathbb{R}$ where $\mu_b(\lambda)$ and $\mu_a(\lambda)$ are the non-negative eigenvalues of $\varrho(\lambda)$. From (3.56) we get that

$$\varrho^t(\lambda) = V^t(\lambda)^*\begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V^t(\lambda) \tag{3.57}$$

for a.e. $\lambda \in \mathbb{R}$ where $V^t(\lambda)$ is the transposed matrix to $V(\lambda)$. Inserting (3.57) into (3.42) we obtain the expression

$$\begin{aligned} &u_{\hat{\varrho}}(x,\lambda) = \\ &\left\langle \begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda)\end{pmatrix} V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix}, V^t(\lambda)\begin{pmatrix} \phi^-(x,\lambda,b) \\ \phi^-(x,\lambda,a)\end{pmatrix}\right\rangle. \end{aligned} \tag{3.58}$$

Let us introduce the unit vectors $e_\tau(\lambda)$,

$$e_\tau(\lambda) = V(\lambda)e_\tau, \quad \tau = b, a \tag{3.59}$$

which perform an orthonormal basis in $\mathbb{C}^2$. We set

$$\begin{aligned} &\vec{\psi}(x,\lambda,e_\tau(\lambda)) := \psi_-(x,\lambda,e_\tau(\lambda)) \oplus \psi(x,\lambda,e_\tau(\lambda)) \oplus \psi_+(x,\lambda,e_\tau(\lambda)) = \\ &\frac{1}{\sqrt{2\pi}}e^{ix\lambda}e_\tau(\lambda) \oplus \frac{1}{\sqrt{2\pi}}(T_*(\lambda)^*e_\tau(\lambda))(x) \oplus \frac{1}{\sqrt{2\pi}}e^{ix\lambda}\Theta_H(\lambda)^*e_\tau(\lambda). \end{aligned} \tag{3.60}$$

Obviously, the system $\{\vec{\psi}(x,\lambda,e_\tau(\lambda))\}_{\tau=b,a}$ performs an orthonormal basis of generalized eigenfunctions. Moreover, a straightforward computation shows that

$$V^t(\lambda)\begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a)\end{pmatrix} = \begin{pmatrix} \psi(x,\lambda,e_b(\lambda)) \\ \psi(x,\lambda,e_a(\lambda))\end{pmatrix} \tag{3.61}$$

which leads to

$$u_{\hat{\varrho}}(x,\lambda) = \mu_b(\lambda)|\psi(x,\lambda,e_b(\lambda))|^2 + \mu_a(\lambda)|\psi(x,\lambda,e_a(\lambda))|^2 \tag{3.62}$$

for $x \in \Omega$ and $\lambda \in \mathbb{R}$.

4 Current density

In accordance with (1.11) the current density $j_{\hat{\varrho}}(x,\lambda)$ for the energy $\lambda \in \mathbb{R}$ is defined by

$$\begin{aligned} j_{\hat{\varrho}}(x,\lambda) \;&:=\; \mu_b(\lambda)\Im\mathrm{m}\left(\tfrac{1}{m(x)}\psi(x,\lambda,e_b(\lambda))'\;\overline{\psi(x,\lambda,e_b(\lambda))}\right) + \\ &\quad\; \mu_a(\lambda)\Im\mathrm{m}\left(\tfrac{1}{m(x)}\psi(x,\lambda,e_a(\lambda))'\;\overline{\psi(x,\lambda,e_a(\lambda))}\right) \end{aligned}, \tag{4.1}$$

$x \in \Omega$, where the eigenfunctions $\psi(x,\lambda,e_\tau(\lambda))$, $\tau = a,b$, are defined by (3.61). We are going to relate the current density to the characteristic function of the maximal dissipative operator H.

Proposition 4.1 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Further, let ϱ be a steady state. Then the current density $j_{\hat{\varrho}}(x,\lambda)$, $x \in \Omega$, $\lambda \in \mathbb{R}$, is independent from x and admits the representation*

$$j_{\hat{\varrho}}(\lambda) = \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)C(\lambda)\right) \tag{4.2}$$

where

$$C(\lambda) := -\frac{1}{2\pi i}\frac{\alpha_a\alpha_b}{\overline{W(\lambda)}}E\Theta_H(\lambda)^* = \frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}\Theta_H(\lambda)E, \tag{4.3}$$

$\lambda \in \mathbb{R}$. Moreover, if $\mathrm{tr}_{\mathbb{C}^2}(\varrho(\cdot)) \in L^1(\mathbb{R})$, then the total current $j_{\hat{\varrho}}$,

$$j_{\hat{\varrho}} := \int_{\mathbb{R}} d\lambda\; j_{\hat{\varrho}}(\lambda), \tag{4.4}$$

is finite and satisfies the estimate

$$|j_{\hat{\varrho}}| \le \frac{1}{2\pi}\int_{\mathbb{R}} d\lambda\; \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)\right) \tag{4.5}$$

Proof. From the definition (4.2) one gets that

$$j_{\hat{\varrho}}(x,\lambda) = \tag{4.6}$$
$$\Im\mathrm{m}\left(\left\langle \begin{pmatrix} \mu_b(\lambda) & 0 \\ 0 & \mu_a(\lambda) \end{pmatrix}\begin{pmatrix} \frac{1}{m(x)}\psi(x,\lambda,e_b(\lambda))' \\ \frac{1}{m(x)}\psi(x,\lambda,e_a(\lambda))' \end{pmatrix}, \begin{pmatrix} \psi(x,\lambda,e_b(\lambda)) \\ \psi(x,\lambda,e_a(\lambda)) \end{pmatrix}\right\rangle\right).$$

Taking into account (3.57) and (3.61) we get

$$j_{\hat{\varrho}}(x,\lambda) = \Im\mathrm{m}\left(\left\langle \varrho^t(\lambda)\begin{pmatrix} \frac{1}{m(x)}\psi^-(x,\lambda,b)' \\ \frac{1}{m(x)}\psi^-(x,\lambda,a)' \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}\right\rangle\right) \tag{4.7}$$

which can be expressed by

$$j_{\hat{\varrho}}(x,\lambda) = \mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)C(x,\lambda)\right) \tag{4.8}$$

where

$$C(x,\lambda) := \qquad (4.9)$$
$$\Im\mathrm{m}\left(\left(\begin{array}{cc} \frac{1}{m(x)}\psi^-(x,\lambda,b)'\,\overline{\psi^-(x,\lambda,b)} & \frac{1}{m(x)}\psi^-(x,\lambda,a)'\,\overline{\psi^-(x,\lambda,b)} \\ \frac{1}{m(x)}\psi^-(x,\lambda,b)'\,\overline{\psi^-(x,\lambda,a)} & \frac{1}{m(x)}\psi^-(x,\lambda,a)'\,\overline{\psi^-(x,\lambda,a)} \end{array}\right)\right)$$

We note that

$$C(x,\lambda) = \frac{1}{i}\left(\begin{array}{cc} W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,b)) & W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,a)) \\ W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,b)) & W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,a)) \end{array}\right) \qquad (4.10)$$

where $W(\cdot,\cdot)$ is the Wronskian defined by (2.5). Since

$$W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,b)) = -\frac{i}{2\pi}\frac{\alpha_b^2\alpha_a^2}{|W(\lambda)|^2} \qquad (4.11)$$

$$W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,b)) = \frac{1}{2\pi}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\left\{W(\lambda) - i\alpha_b^2 v_a(b,\lambda)\right\} \qquad (4.12)$$

$$W(\overline{\psi^-(x,\lambda,b)},\psi^-(x,\lambda,a)) = -\frac{1}{2\pi}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\left\{W(\lambda) - i\alpha_a^2 v_b(a,\lambda)\right\} \qquad (4.13)$$

$$W(\overline{\psi^-(x,\lambda,a)},\psi^-(x,\lambda,a)) = \frac{i}{2\pi}\frac{\alpha_a^2\alpha_b^2}{|W(\lambda)|^2} \qquad (4.14)$$

we find

$$C(x,\lambda) = \frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\left(\begin{array}{cc} -i\alpha_b\alpha_a & -(W(\lambda) - i\alpha_a^2 v_b(a,\lambda)) \\ W(\lambda) - i\alpha_b^2 v_a(b,\lambda) & i\alpha_a\alpha_b \end{array}\right). \qquad (4.15)$$

This yields

$$C(x,\lambda) = \qquad (4.16)$$
$$-\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{|W(\lambda)|^2}\left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array}\right)\left(\begin{array}{cc} W(\lambda) - i\alpha_b^2 v_a(b,\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & W(\lambda) - i\alpha_a^2 v_b(a,\lambda) \end{array}\right).$$

From (2.21) we obtain

$$\Theta_H(\lambda)^* = \frac{1}{\overline{W(\lambda)}}\left(\begin{array}{cc} W(\lambda) - i\alpha_b^2 v_a(b,\lambda) & i\alpha_b\alpha_a \\ i\alpha_b\alpha_a & W(\lambda) - i\alpha_a^2 v_b(a,\lambda) \end{array}\right). \qquad (4.17)$$

Hence, one has

$$C(x,\lambda) = -\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}E\Theta_H(\lambda)^* \qquad (4.18)$$

where

$$E := \left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array}\right). \qquad (4.19)$$

This shows that $C(x,\lambda)$ is actually independent of $x \in \Omega$. By (4.8) this leads to the representation

$$j_{\hat{\varrho}}(x,\lambda) = -\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)}\mathrm{tr}_{\mathbb{C}^2}\left(\varrho(\lambda)E\Theta_H(\lambda)^*\right) \qquad (4.20)$$

which shows that the current density is also independent of $x \in \Omega$. Thus it makes sense to denote $C(x,\lambda)$ and $j_{\hat{e}}(x,\lambda)$ by $C(\lambda)$ and $j_{\hat{e}}(\lambda)$, respectively. Hence, we have proved one part of the assertion (4.2) and (4.3). Taking into account the identity

$$\frac{1}{\overline{W(\lambda)}} E\Theta_H(\lambda)^* = -\frac{1}{W(\lambda)}\Theta_H(\lambda)E \tag{4.21}$$

we verify the other part.

It remains to show (4.4) and (4.5). To this end we note that from (4.17) one gets

$$J\Theta_H(\lambda)^* = J + \frac{i}{W(\lambda)}\begin{pmatrix} \alpha_b\alpha_a & -\alpha_a^2 v_b(a,\lambda) \\ -\alpha_b^2 v_a(b,\lambda) & \alpha_b\alpha_a \end{pmatrix} \tag{4.22}$$

where

$$J := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.23}$$

Hence we find

$$\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*) = 2i\frac{\alpha_b\alpha_a}{W(\lambda)} \tag{4.24}$$

which yields

$$\frac{1}{2\pi i}\frac{\alpha_b\alpha_a}{W(\lambda)} = -\frac{1}{4\pi}\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*). \tag{4.25}$$

Using the definition (4.3) we finally obtain

$$j_{\hat{e}}(\lambda) = -\frac{1}{4\pi}\mathrm{tr}_{\mathbb{C}^2}(J\Theta_H(\lambda)^*)\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)\Theta_H(\lambda)E). \tag{4.26}$$

This leads to the estimate

$$|j_{\hat{e}}(\lambda)| \le \frac{1}{4\pi}\|\Theta_H(\lambda)^*\|_{\mathcal{L}_1(\mathbb{C}^2)}\|\varrho(\lambda)\|_{\mathcal{L}_1(\mathbb{C}^2)}. \tag{4.27}$$

Since $\|\Theta_H(\lambda)^*\|_{\mathcal{L}_1(\mathbb{C}^2)} \le 2$ and $\|\varrho(\lambda)\|_{\mathcal{L}_1(\mathbb{C}^2)} = \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda))$ we find

$$|j_{\hat{e}}(\lambda)| \le \frac{1}{2\pi}\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)) \tag{4.28}$$

which immediately proves (4.5). □

In correspondence to the carrier density it seems to be useful to introduce the following definition.

Definition 4.2 Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. Then the matrix $C(\lambda)$ and the value $j_\varrho(\lambda)$ are called the current density observable and the current density at energy $\lambda \in \mathbb{R}$ of the system described by H, respectively.

The definition is again justified by the fact that the current density at energy $\lambda \in \mathbb{R}$ is the expectation value of the current density observable at energy $\lambda \in \mathbb{R}$, i.e. $j_{\hat{\varrho}}(\lambda) = \mathbb{E}_{\varrho(\lambda)}(C(\lambda))$ for $\lambda \in \mathbb{R}$. Using this notation formula (4.4) takes the form

$$j_{\hat{\varrho}} = \int_{\mathbb{R}} d\lambda \; \mathbb{E}_{\varrho(\lambda)}(C(\lambda)). \tag{4.29}$$

In the following corollary we consider the case that the steady state ϱ is a function of K, i.e.

$$\varrho = f(K), \tag{4.30}$$

where, of course, $f(\cdot) \in L^\infty(\mathbb{R})$ and $f(\lambda) \geq 0$ for a.e. $\lambda \in \mathbb{R}$ and. In this case the density matrix ϱ belongs to the bicommutant of K.

Corollary 4.3 *Assume $m + \frac{1}{m} \in L^\infty([a,b])$, $V \in L^2([a,b])$ and $\kappa_a, \kappa_b \in \mathbb{C}_+$. If the steady state ϱ is given by (4.30) with a non-negative function $f(\cdot) \in L^\infty(\mathbb{R})$, then $j_{\hat{\varrho}}(\lambda) = 0$ for a.e. $\lambda \in \mathbb{R}$.*

Proof. In this case one has

$$\varrho(\lambda) = f(\lambda) I_{\mathbb{C}^2}, \quad \lambda \in \mathbb{R}. \tag{4.31}$$

which gives

$$j_{\hat{\varrho}}(\lambda) = f(\lambda)\mathrm{tr}(C(\lambda)) = -\frac{1}{2\pi i} f(\lambda) \frac{\alpha_b \alpha_a}{W(\lambda)} \mathrm{tr}_{\mathbb{C}^2}(E\Theta_H(\lambda)^*). \tag{4.32}$$

By (4.17) we immediately get that $\mathrm{tr}_{\mathbb{C}^2}(E\Theta_H(\lambda)^*) = 0$ for $\lambda \in \mathbb{R}$. □

If the steady state ϱ has the form

$$\varrho(\lambda) = \begin{pmatrix} \varrho^{bb}(\lambda) & 0 \\ 0 & \varrho^{aa}(\lambda) \end{pmatrix}, \tag{4.33}$$

then the current density is given by

$$j_{\hat{\varrho}}(\lambda) = -\frac{1}{2\pi} \frac{\alpha_a^2 \alpha_b^2}{|W(\lambda)|^2} (\varrho^{bb}(\lambda) - \varrho^{aa}(\lambda)). \tag{4.34}$$

This current density is different from zero if $\varrho^{bb}(\lambda) \neq \varrho^{aa}(\lambda)$ at least for a set of positive Lebesgue measure. So a current density different from zero arises only if we have a occupation disparity between the two eigenstates $\psi^-(x,\lambda,b)$ and $\psi^-(x,\lambda,a)$. This is the case if the steady state ϱ belongs to the commutant of K but not to the bicommutant. In other words, the density matrix (1.8) used for self-adjoint boundary conditions and generalized by (4.30) to the dissipative case leads to a zero current density.

5 Remarks

1. The carrier density $u_{\hat{\varrho}}(\cdot)$ performed by (3.41) and (3.44) is a straightforward generalization of the corresponding definition (1.5) of the carrier density in the self-adjoint case. Indeed, this correspondence relies on the replacements

$$\begin{array}{rcl} l & \longleftrightarrow & \{a, b, \lambda\}, \\ \{\psi_l\}_{l=1}^{\infty} & \longleftrightarrow & \{\vec{\psi}(\cdot, \lambda, \tau)\}_{\lambda\in\mathbb{R},\tau=a,b}, \\ \sum_{l=1}^{\infty} & \longleftrightarrow & \int_{\lambda\in\mathbb{R}} d\lambda \ \sum_{\tau=a,b} \\ \varrho_l & \longleftrightarrow & \varrho(\lambda) \end{array} \tag{5.1}$$

The same holds for the current density defined by (4.1) which is a straightforward generalization of (1.11). *However, in contrast to the self-adjoint case the current density now is not necessarily zero!*

2. There is consensus in the conviction that scattering states are responsible for the current. This usually leads to a a relation between current density and scattering matrix. Actually, the same takes place here. Formulae (4.2) and (4.3) relate the current density $j_{\hat{\varrho}}(\lambda)$ with the characteristic function $\Theta_{H^*}(\lambda)$ of H^*. It turns out that the characteristic function $\Theta_{H^*}(\lambda)$ of H^* can be regarded as the scattering matrix of an associated scattering system. Indeed, with the self-adjoint dilation K one can associate a so-called Lax-Phillips scattering theory [2, 16]. To this end one introduces the Hilbert space $\mathfrak{K}_0$,

$$\mathfrak{K}_0 := L^2(\mathbb{R}, \mathbb{C}^2) = \mathcal{D}_- \oplus \mathcal{D}_+ \subseteq \mathfrak{K}. \tag{5.2}$$

and the identification operators $J_\pm : \mathfrak{K}_0 \longrightarrow \mathfrak{K}$,

$$\begin{array}{rcl} \vec{f} = J_- f & := & P^{\mathfrak{K}_0}_{\mathcal{D}_-} f \oplus 0 \oplus 0, \quad f \in \mathfrak{K}_0, \\ \vec{f} = J_+ f & := & 0 \oplus 0 \oplus P^{\mathfrak{K}_0}_{\mathcal{D}_+} f, \quad f \in \mathfrak{K}_0. \end{array} \tag{5.3}$$

The subspaces $\mathcal{D}_-$ and $\mathcal{D}_+$ are called incoming and outgoing subspaces, respectively. On the Hilbert space $\mathfrak{K}_0$ one defines the self-adjoint operator K_0,

$$(K_0 f)(x) = -i\frac{d}{dx} f(x) \tag{5.4}$$

with the domain $\mathrm{dom}(K_0) := W^{1,2}(\mathbb{R}, \mathbb{C}^2)$. The Lax-Phillips wave operators

$$W_\pm = s - \lim_{t\to\pm\infty} e^{itK} J_\pm e^{-itK_0} \tag{5.5}$$

exist and are complete, i.e. $\mathrm{ran}(W_\pm) = \mathfrak{K}$. The corresponding Lax-Phillips scattering operator $S = W_+^* W_- : \mathfrak{K}_0 \longrightarrow \hat{\mathfrak{K}}$, is unitary and commutes with the self-adjoint operator K_0. By $\mathcal{F} : \mathfrak{K}_0 \longrightarrow \hat{\mathfrak{K}}$ we denote the Fourier transform

$$(\mathcal{F}f)(\lambda) = \hat{f}(\lambda) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dx \ e^{-i\lambda x} f(x), \quad f \in \mathfrak{K}_0, \quad \lambda \in \mathbb{R}. \tag{5.6}$$

We note that $\mathcal{F}K_0\mathcal{F}^{-1} = M$ where M is defined by (2.43). Since S commutes with K_0 the operator $\hat{S} = \mathcal{F}S\mathcal{F}^{-1} : \hat{\mathfrak{K}} \longrightarrow \hat{\mathfrak{K}}$ commutes with M. Hence $\hat{S}$ is a multiplication operator given by

$$(\hat{S}\hat{f})(\lambda) = S(\lambda)\hat{f}(\lambda), \quad \hat{f} \in \hat{\mathfrak{K}}, \quad \lambda \in \mathbb{R}, \tag{5.7}$$

where $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of unitary operators which is called the Lax-Phillips scattering matrix. A rather involved computation shows that

$$S(\lambda) = \Theta_{H^*}(\lambda) \tag{5.8}$$

for a.e. $\lambda \in \mathbb{R}$, see for example [1]. By the way one has

$$\Phi_- = \mathcal{F}W_+^* \quad \text{and} \quad \Phi_+ = \mathcal{F}W_-^* \tag{5.9}$$

where is Φ_- is the incoming Fourier transformation, cf. (2.41) and (2.42), and Φ_+ is the so-called outgoing Fourier transform which was introduced in [12].

3. As mentioned above the quantity $N_\varrho(\omega)$,

$$N_\varrho(\omega) := \|u_{\hat{\varrho}}\|_{L^1(\omega)} = \int_\omega dx\; u_{\hat{\varrho}}(x), \tag{5.10}$$

has the meaning of the number of carriers on the Borel set subset $\omega \subseteq \Omega = [a, b]$. By (3.44) one has the representation

$$N_\varrho(\omega) = \mathrm{tr}(\varrho U(\omega)). \tag{5.11}$$

Obviously $N := N_\varrho(\Omega)$ is the total number of carriers on the interval $[a, b]$. We note that under the condition(3.23) by Proposition 3.7 the total number of carriers in Ω is always finite.

In accordance with [15] the time evolution of the density matrix ϱ is given by

$$\varrho(t) = e^{-itK}\varrho e^{itK}, \quad t \in \mathbb{R}. \tag{5.12}$$

Hence, the number of particles at time $t \in \mathbb{R}$ on ω is given by

$$N_{\varrho(t)}(\omega) := \mathrm{tr}(\varrho(t)U(\omega)), \quad t \in \mathbb{R}. \tag{5.13}$$

Since ϱ commutes with K one has $\varrho(t) = \varrho$ and $N_{\varrho(t)}(\omega) = N_\varrho(\omega)$ or

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = 0, \quad \omega \subseteq \Omega, \quad t \in \mathbb{R}. \tag{5.14}$$

If the condition

$$C_{\hat{\varrho}} := \sup_{\lambda\in\mathbb{R}}(1 + \lambda^2)\|\varrho(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty \tag{5.15}$$

is satisfied, then

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \tag{5.16}$$
$$-i\mathrm{tr}(K\varrho(t)U(\omega)) + i\mathrm{tr}(\varrho(t)KU(\omega)) = -i\mathrm{tr}(K\varrho U(\omega)) + i\mathrm{tr}(\varrho KU(\omega)).$$

Hence

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \tag{5.17}$$
$$-i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \lambda\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) + i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \lambda\ \mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)).$$

By formula (3.42) we find

$$\int_{\omega} dx\ \lambda(\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) = \tag{5.18}$$
$$\int_{\omega} dx\ \lambda \left\langle \varrho^t(\lambda) \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle.$$

Since $l(\psi^-(x,\lambda,\tau)) = \lambda\psi^-(x,\lambda,\tau)$ one gets

$$\int_{\omega} dx\ \lambda(\mathrm{tr}_{\mathbb{C}^2}(\varrho(\lambda)D(x,\lambda)) = \tag{5.19}$$
$$\int_{\omega} dx\ \left\langle \varrho^t(\lambda) \begin{pmatrix} l(\psi^-(x,\lambda,b)) \\ l(\psi^-(x,\lambda,a)) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle.$$

Hence

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \tag{5.20}$$
$$-i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \left\langle \varrho^t(\lambda) \begin{pmatrix} l(\psi^-(x,\lambda,b)) \\ l(\psi^-(x,\lambda,a)) \end{pmatrix}, \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix} \right\rangle +$$
$$i\int_{\mathbb{R}} d\lambda \int_{\omega} dx\ \left\langle \varrho^t(\lambda) \begin{pmatrix} \psi^-(x,\lambda,b) \\ \psi^-(x,\lambda,a) \end{pmatrix}, \begin{pmatrix} l(\psi^-(x,\lambda,b)) \\ l(\psi^-(x,\lambda,a)) \end{pmatrix} \right\rangle$$

Let $\omega = [c,d] \subseteq [a,b]$. Integrating by parts and taking into account formula (4.7) we get

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = \int_{\mathbb{R}} d\lambda\ \{j_{\hat{\varrho}}(c,\lambda) - j_{\hat{\varrho}}(d,\lambda)\}. \tag{5.21}$$

The total current $j_{\hat{\varrho}}(x)$ at the point $x \in [a,b]$ is defined by

$$j_{\hat{\varrho}}(x) := \int_{\mathbb{R}} d\lambda\ j_{\hat{\varrho}}(x,\lambda). \tag{5.22}$$

This yields This yields

$$\frac{d}{dt}N_{\varrho(t)}(\omega) = j_{\hat{\varrho}}(c) - j_{\hat{\varrho}}(d) \tag{5.23}$$

which shows that the change of the number of carriers in the set $[c,d]$ is equal to the difference between the incoming current $j_{\hat{\varrho}}(c)$ at point c and the outgoing current $j_{\hat{\varrho}}(d)$ at point d which very well corresponds to the physical intuition. Since by Proposition 4.1 the current density $j_{\hat{\varrho}}(x,\lambda)$ does not depend on $x \in [a,b]$ one gets

$j_{\hat{\varrho}}(d) = j_{\hat{\varrho}}(c)$ which again verifies (5.14). The relation (5.23) is the integral form of the so-called continuity equation which has the differential form

$$\frac{\partial}{\partial t} u_{\hat{\varrho}(t)}(x) + \frac{\partial}{\partial x} j_{\hat{\varrho}(t)}(x) = 0, \quad t \in \mathbb{R}, \quad x \in \Omega, \tag{5.24}$$

where $u_{\hat{\varrho}(t)}(x)$ is the carrier density at time $t \in \mathbb{R}$ and $j_{\varrho(t)}(x)$ is current density at time t given by (5.22). Since $u_{\hat{\varrho}(t)}(x) = u_{\hat{\varrho}}(x)$ is independent of t and $j_{\varrho(t)}(x)$ is independent of x the continuity equation (5.24) obviously holds in the present situation.

4. On the basis of the considerations above we are able to give a mathematically rigourous foundation of dissipative Schrödinger-Poisson systems. To this end we consider different species $\pm$ of particles (holes and electrons) and assume that that for these species the effective masses $m_\pm$, external potentials $V_0^\pm$ and coefficients $\kappa_a^\pm, \kappa_b^\pm \in \mathbb{C}_+$ are given. For each species this leads to different dissipative Schrödinger operators $H^\pm(V_\pm)$ defined in accordance with (1.12), (2.1) and (2.2). The potential V entering into the definition of the Schrödinger operators is different for different species. It takes the form

$$V_\pm := V_0^\pm \pm \varphi(u). \tag{5.25}$$

where the electrostatic potential φ is a solution of the Poisson equation (1.1) with boundary condition (1.3). The carrier densities $u^\pm$ entering into Poisson's equation are obtained from the dissipative Schrödinger operators $H^\pm(V_\pm)$ in accordance with Section 3. To this end we assume that the families of matrices $\{\varrho_\pm(\lambda)\}_{\lambda\in\mathbb{R}}$, which obey

$$C_{\hat{\varrho}_\pm} := \sup_{\lambda\in\mathbb{R}} \sqrt{\lambda^2+1}\|\varrho_\pm(\lambda)\|_{\mathcal{B}(\mathbb{C}^2)} < \infty, \tag{5.26}$$

are given and we define the carrier densities $u^\pm(x) := u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x)$ in accordance with Section 3, i.e., if $D^\pm(V_\pm)(x)$ are the carrier density observables at $x \in \Omega$ and at energy $\lambda \in \mathbb{R}$, then the carrier densities are computed by

$$u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x) = \int_{\mathbb{R}} d\lambda \; u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x,\lambda), \quad x \in \Omega, \tag{5.27}$$

where

$$u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x,\lambda) = \mathrm{tr}_{\mathbb{C}^2}(\varrho_\pm(\lambda) D^\pm(V_\pm)(x,\lambda)), \quad x \in \Omega, \quad \lambda \in \mathbb{R}. \tag{5.28}$$

Moreover, if $\mathrm{tr}_{\mathbb{C}^2}(\varrho_\pm(\cdot)) \in L^1(\mathbb{R})$ is valid, then the current densities $j^\pm_{\hat{\varrho}_\pm}$,

$$j^\pm_{\hat{\varrho}_\pm} = \int_{\mathbb{R}} d\lambda \; j^\pm_{\hat{\varrho}_\pm}(V_\pm)(\lambda) \tag{5.29}$$

are also well-defined and finite, cf. Section 4. The so described system is called a dissipative Schrödinger-Poisson system. We note that the total number of carriers $N^\pm(V_\pm)$ is given by

$$N^\pm(V_\pm) = \int_\Omega dx \; u^\pm_{\hat{\varrho}_\pm}(V_\pm)(x) \tag{5.30}$$

and is not fixed.

In a forthcoming paper [13] we show that under suitable conditions on $\epsilon(\cdot)$, $C(\cdot)$, $m_\pm(\cdot)$, $V_0^\pm(\cdot)$, $\kappa_b^\pm$, $\kappa_a^\pm$ and $\varrho_\pm$ this dissipative Schrödinger-Poisson system always admits a self-consistent solution.

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