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Dissipative Schrödinger-type operator as a model for generation and recombination

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Abstract

Non-selfadjoint operators play an important role in the modeling of open quantum systems. We consider a one-dimensional Schrödinger-type operator of the form

$$-\frac{1}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx}+V-\sum\kappa_j\delta(\cdot-x_j),\quad \mathrm{Im}(\kappa_j)>0,$$

with dissipative boundary conditions. An explicit description of the characteristic function, the minimal dilation and the generalized eigenfunctions of the dilation is given. The quantities of carrier and current densities are rigorously defined. Furthermore we will show that the current is not constant and that the variation of the current depend essentially on the chosen density matrix and the imaginary parts of the delta potentials, i.e. $\mathrm{Im}(\kappa_j)$. This correspondence can be used to model a recombination-generation rate in the open quantum system.

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Contents

1 Introduction

To embed a quantum mechanically described structure into a macroscopic flow, one has to replace the selfadjoint boundary conditions by non-selfadjoint ones [KNR01a, Fre90, BA98, BADM97]. This leads to so-called open quantum systems. One-dimensional Schrödinger-type operators with dissipative boundary conditions have been intensely studied in [KNR01b]. We extend the model used there by adding dissipative delta perturbations, i.e. we consider an operator formally given by

$$H = -\frac{1}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx} + \tilde{V}, \tag{1.1}$$

where

$$\tilde{V}(\cdot) = V(\cdot) - \sum_{j=1}^{N} \kappa_j \delta(\cdot - x_j), \tag{1.2}$$

$x_j \in (a,b)$, $x_j \neq x_i$ for $i \neq j$, and $\kappa_j \in \mathbb{C}_+ := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) > 0\}$. The potential V is assumed to be a real-valued $\mathsf{L}^2([a,b])$-function and the effective mass $m > 0$ satisfies $m, \frac{1}{m} \in \mathsf{L}^\infty(a,b)$. Point interactions of this kind are extensively studied in the literature for self-adjoint boundary conditions and real coupling constants κ_j, cf. [AGHH88, AK00] and references therein. Since the boundary conditions are not self-adjoint and the coupling constant are complex the expression (1.1)-(1.2) generates a maximal dissipative operator, see below. Such operators naturally arises if one is interested in mathematical models for semiconductor devices with recombination and generation processes of carriers which are embedded in a macrostructure. This case is not treated in [AGHH88] and [AK00]. To analyze such operators it is fruitful to use the dilation theory for maximal dissipative operators [FN70, D80]. To Schrödinger operators this approach was specified in [P77, P76, P84, P96, P99], see also [A87, A88, A89, A90, A93, A97]. In [KNR01c] this approach was used to define quantities such as steady states, carrier and current density for devices without recombination and generation. In the present article we modified this approach to fit our situation, i.e. where recombination and generation processes are included.

In an one-dimensional drift-diffusion model (cf. [S84, M86, MRS90, J01]) the macroscopic flow is modeled by the continuity equations

$$\begin{aligned} \tfrac{\partial}{\partial t}n(x,t) - \tfrac{\partial}{\partial x}J_n(x,t) &= -R(n,p), \\ \tfrac{\partial}{\partial t}p(x,t) + \tfrac{\partial}{\partial x}J_p(x,t) &= -R(n,p), \end{aligned} \tag{1.3}$$

where n, p denote the electron and hole densities, J_n, J_p the corresponding currents and $R(n,p)$ the recombination-generation rate. The stationary continuity equation is given by equation (1.3), where $\frac{\partial}{\partial t}n(x,t) = \frac{\partial}{\partial t}p(x,t) = 0$ and $J_k(x,t) = J_k(x)$, $k = n, p$. Replacing carrier densites n, p and current densities J_n, J_p by quantum mechanical expressions like [KNR01c] we are able to include recombination-generation effects into the open quantum system determined by (1.1) and (1.2) and to preserve the form of the continuity equations (1.3) for the quantum mechanically described structure. However, this implies that one has to chosen the imaginary parts of the coupling constants κ_j in an appropriate manner. We outline how the imaginary parts has to be chosen. In forthcoming papers we have the aim to consider a dissipative Schrödinger-Poisson [BKNR02a] system with recombination and generation effects.

The paper is organized as follows: In section 2 we rigorously define the dissipative Schrödinger-type operator and show that the operator H is maximal dissipative. We use the well-know dilation theory as a main tool for our investigations. Therefore, the characteristic function and the minimal dilation corresponding to the maximal dissipative operator are the main objective in the sections 3 and 4. Section 5 is devoted to the generalized eigenfunctions of the dilation operator. In the sections 6 and 7 we give a definition of the density matrix and define the quantities of carrier and current densities in terms of the generalized eigenfunctions of the dilation (cf. [KNR01c]). The motivation for this definition is, that the selfadjoint dilation is regarded as the Hamiltonian of a larger closed system which contains the open system given by the dissipative operator H. In section 8 we show that, depending on the density matrix, loss and/or gain effect of the open system can be achieved. We close with some remarks and a discussion on how the imaginary parts of the delta potentials have to be chosen in order to include recombination-generation processes within the open quantum model.

2 Dissipative Schrödinger operators

Let x_j, $j = 1, \cdots, N$, be numbers contained in the bounded interval $\Omega := (a,b) \subset \mathbb{R}$, such that $a < x_1 < x_2 < \cdots < x_N < b$. Furthermore let $V \in \mathsf{L}^2(a,b)$ be real-valued, and $m \in \mathsf{L}^\infty(a,b)$, with $m > 0$ and $\frac{1}{m} \in \mathsf{L}^\infty(a,b)$. In accordance with [KNR01b] we define the sesquilinear form

$$\begin{aligned}\mathfrak{t}[u,v] := &\int_a^b \frac{1}{2}\frac{1}{m(x)} u(x)\overline{v(x)} + V(x)u(x)\overline{v(x)}dx \\ &- \kappa_a u(a)\overline{v(a)} - \sum_{j=1}^N \kappa_j u(x_j)\overline{v(x_j)} - \kappa_b u(b)\overline{v(b)},\end{aligned}$$

for $u, v \in \mathsf{D}(\mathfrak{t}) = \mathsf{W}^{1,2}(a,b)$ and $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+ := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) > 0\}$. Mimicking the proof of Theorem 2.20 in [KNR01a], we get that the form $\mathfrak{t}$ is closed on $\mathcal{H} = \mathsf{L}^2(a,b)$ and sectorial. Thus we get the existence of a maximal sectorial operator H, such that $(Hf, v) = \mathfrak{t}[f,v]$ for all $f \in \mathsf{D}(H)$ and $v \in \mathsf{D}(\mathfrak{t})$. It can be shown that the operator H is given by

$$\mathsf{D}(H) = \left\{ f \in \mathsf{W}^{1,2}(a,b) \;\middle|\; \begin{array}{l} \frac{1}{m}f' \in \mathsf{W}^{1,2}(a,x_1) \oplus \bigoplus_{j=1}^{N-1} \mathsf{W}^{1,2}(x_j,x_{j+1}) \oplus \mathsf{W}^{1,2}(x_N,b), \\ \frac{1}{2m(a)}f'(a) = -\kappa_a f(a),\ \frac{1}{2m(b)}f'(b) = \kappa_b f(b) \\ \frac{1}{2m(x_j+0)}f'(x_j+0) - \frac{1}{2m(x_j-0)}f'(x_j-0) = -\kappa_j f(x_j), \\ \forall j = 1, \cdots, N \end{array} \right\},$$

and

$$(Hf)(x) = (l(f))(x), \quad f \in \mathsf{D}(H),$$

where

$$(l(f))(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x) + V(x)f(x).$$

Since $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$, the operator H is dissipative, i.e. $\mathrm{Im}(Hf,f) \le 0$, $f \in \mathsf{D}(H)$. This can be seen by

$$\mathrm{Im}(Hf,f) = \mathrm{Im}\ \mathfrak{t}[f,f] = -\frac{\alpha_a^2}{2}|f(a)|^2 - \frac{\alpha_b^2}{2}|f(b)|^2 - \sum_{j=1}^N \frac{\alpha_j^2}{2}|f(x_j)|^2,$$

where $\kappa_a = q_a + \frac{i\alpha_a^2}{2}, \cdots, \kappa_b = q_b + \frac{i\alpha_b^2}{2}$, for some $q_a, \cdots, q_b, \alpha_a, \cdots, \alpha_b \in \mathbb{R}$, $\alpha_a, \cdots, \alpha_b > 0$. A dissipative operator is called maximal dissipative, if it does not admit any proper dissipative extension. Since H is maximal sectorial it is also maximal dissipative. Furthermore, H is purely maximal dissipative (cf. [KNR01a]), i.e. it has no selfadjoint part [FN70]. This implies that H has no real eigenvalues.

Let us introduce some notions. For simplicity we will occasional write $a = x_0$, $\kappa_a = \kappa_0$, $\alpha_a = \alpha_0$, $b = x_{N+1}$, $\kappa_b = \kappa_{N+1}$, and $\alpha_b = \alpha_{N+1}$. We set

$$\Delta(g,f)(x) := \frac{1}{2m(x+0)}g'(x+0) - \frac{1}{2m(x-0)}f'(x-0), \quad \Delta(g)(x) := \Delta(g,g)(x).$$

For a matrix $A = (a_{ij})$, with $a_{ij} \in \mathbb{C}$, $\overline{A}$ will denote the matrix in which every element is complex conjugated, i.e. $\overline{A} = (\overline{a}_{ij})$.

In order to get an explicit description of the resolvent of H we introduce the elementary solutions $v_a(x,z)$ and $v_b(x,z)$ defined by

$$\begin{aligned}
&l(v_a(\cdot,z))(x) - zv_a(x,z) = 0,\ v_a(a,z) = 1,\ \tfrac{1}{2m(a)}v_a'(a,z) = -\kappa_a,\\
&\Delta(v_a(\cdot,z))(x_j) = -\kappa_j v_a(x_j,z), \quad \forall j = 1,\cdots,N,
\end{aligned}$$

$$\begin{aligned}
&l(v_b(\cdot,z))(x) - zv_b(x,z) = 0,\ v_b(b,z) = 1,\ \tfrac{1}{2m(b)}v_b'(b,z) = \kappa_b,\\
&\Delta(v_b(\cdot,z))(x_j) = -\kappa_j v_b(x_j,z), \quad \forall j = 1,\cdots,N.
\end{aligned}$$

The existence of these solutions can be proven as in [KNR01b].

The Wronskian of $v_a(x,z)$ and $v_b(x,z)$ is defined by

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

We note that $W(v_a(\cdot,z),v_b(\cdot,z))(x)$ is constant for $x \in (x_i,x_{i+1})$. Furthermore, one easily checks that

$$W(v_a(\cdot,z),v_b(\cdot,z))(x_i - 0) = W(v_a(\cdot,z),v_b(\cdot,z))(x_i + 0).$$

Thus we write $W(z) := W(v_a(\cdot,z),v_b(\cdot,z))(x)$.

The functions defined by

$$v_{*a}(x,z) := \overline{v_a(x,\overline{z})}, \qquad \text{and} \qquad v_{*b}(x,z) := \overline{v_b(x,\overline{z})},$$

are solutions of

$$\begin{aligned}
&l(v_{*a}(\cdot,z))(x) - zv_{*a}(x,z) = 0,\ v_{*a}(a,z) = 1,\ \tfrac{1}{2m(a)}v_{*a}'(a,z) = -\overline{\kappa_a}\\
&\Delta(v_{*a}(\cdot,z))(x_j) = -\overline{\kappa_j} v_{*a}(x_j,z), \quad \forall j = 1,\cdots,N,
\end{aligned}$$

$$\begin{aligned}
&l(v_{*b}(\cdot,z))(x) - zv_{*b}(x,z) = 0,\ v_{*b}(b,z) = 1,\ \tfrac{1}{2m(b)}v_{*b}'(b,z) = \overline{\kappa_b}\\
&\Delta(v_{*b}(\cdot,z))(x_j) = -\overline{\kappa_j} v_{*b}(x_j,z), \quad \forall j = 1,\cdots,N.
\end{aligned}$$

Obviously, the Wronskian $W_*(z) := W(v_{*a}(\cdot,z),v_{*b}(\cdot,z))(x)$ satisfies $W_*(z) = \overline{W(\overline{z})}$.

We are now able to write the resolvents of H and H^* as integral operators, where the kernels are given in terms of the elementary solutions (see also [K80]).

Theorem 2.1 *Let $V \in \mathsf{L}^2(a,b)$ be real valued and $\kappa_a,\kappa_1,\cdots,\kappa_N,\kappa_b \in \mathbb{C}_+$. Then the resolvent of the maximal dissipative operator H is given by*

$$((H-z)^{-1}f)(x) = -\frac{v_b(x,z)}{W(z)}\int_a^x v_a(y,z)f(y)\,dy - \frac{v_a(x,z)}{W(z)}\int_x^b v_b(y,z)f(y)\,dy, \tag{2.1}$$

for $f \in \mathcal{H}$ and $z \in \varrho(H)$.

The resolvent of the adjoint operator H^* admits the representation

$$((H^*-z)^{-1}f)(x) = -\frac{v_{*b}(x,z)}{W_*(z)}\int_a^x v_{*a}(y,z)f(y)\,dy - \frac{v_{*a}(x,z)}{W_*(z)}\int_x^b v_{*b}(y,z)f(y)\,dy, \tag{2.2}$$

for $f \in \mathcal{H}$ and $z \in \varrho(H^*)$.

We omit the proof, but note that $W(z) = 0 \Leftrightarrow z \in \sigma(H)$ and $W_*(z) = 0 \Leftrightarrow z \in \sigma(H^*)$, where $\sigma(\cdot)$ denotes the spectrum of the corresponding operator.

3 The characteristic function

We define the unclosed operator $\alpha : \mathcal{H} \to \mathbb{C}^{N+2}$ by

$$\alpha f = \begin{pmatrix} \alpha_b f(b) \\ -\alpha_N f(x_N) \\ \vdots \\ -\alpha_1 f(x_1) \\ -\alpha_a f(a) \end{pmatrix}, \quad \mathsf{D}(\alpha) = \mathsf{C}(a,b).$$

Let us introduce the operator valued function $T(z) : \mathcal{H} \to \mathbb{C}^{N+2}$ given by

$$T(z)f := \alpha(H - z)^{-1} f, \tag{3.1}$$

for $f \in \mathcal{H}$ and $z \in \varrho(H)$. Using the expression (2.1) we get

$$T(z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b v_a(y,z) f(y)\, dy \\ \alpha_N v_b(x_N,z) \int_a^{x_N} v_a(y,z) f(y)\, dy + \alpha_N v_a(x_N,z) \int_{x_N}^b v_b(y,z)\, dy \\ \vdots \\ \alpha_1 v_b(x_1,z) \int_a^{x_1} v_a(y,z) f(y)\, dy + \alpha_1 v_a(x_1,z) \int_{x_1}^b v_b(y,z)\, dy \\ \alpha_a \int_a^b v_b(y,z) f(y)\, dy \end{pmatrix}.$$

The adjoint operator $T(z)^*$ is given by

$$\begin{aligned} (T(z)^*\xi)(x) = &\frac{1}{W_*(\overline{z})}\{-\alpha_b v_{*a}(x,\overline{z})\xi^b \\ &+ \alpha_N (v_{*b}(x_N,\overline{z}) v_{*a}(x,\overline{z}) \chi_{[a,x_1)}(x) + v_{*a}(x_N,\overline{z}) v_{*b}(x,\overline{z}) \chi_{[x_N,b]})\xi^N \\ &\vdots \\ &+ a_1 (v_{*b}(x_1,\overline{z}) v_{*a}(x,\overline{z}) \chi_{[a,x_1)}(x) + v_{*a}(x_1,\overline{z}) v_{*b}(x,\overline{z}) \chi_{[x_1,b]})\xi^1 \\ &+ \alpha_a v_{*b}(x,\overline{z})\xi^a\}, \end{aligned}$$

for $x \in [a,b]$, where

$$\xi = \begin{pmatrix} \xi^b \\ \xi^N \\ \vdots \\ \xi^1 \\ \xi^a \end{pmatrix} \in \mathbb{C}^{N+2}. \tag{3.2}$$

Similarly, we define $T_*(z) : \mathcal{H} \to \mathbb{C}^{N+2}$ by

$$T_*(z)f := \alpha(H^* - z)^{-1} f,$$

for $f \in \mathcal{H}$ and $z \in \varrho(H)$. Using equation (2.2) one gets

$$T_*(z)f = \frac{1}{W(z)} \begin{pmatrix} -\alpha_b \int_a^b v_{*a}(y,z) f(y)\, dy \\ \alpha_N v_{*b}(x_N,z) \int_a^{x_N} v_{*a}(y,z) f(y)\, dy + \alpha_N v_{*a}(x_N,z) \int_{x_N}^b v_{*b}(y,z)\, dy \\ \vdots \\ \alpha_1 v_{*b}(x_1,z) \int_a^{x_1} v_{*a}(y,z) f(y)\, dy + \alpha_1 v_{*a}(x_1,z) \int_{x_1}^b v_{*b}(y,z)\, dy \\ \alpha_a \int_a^b v_{*b}(y,z) f(y)\, dy \end{pmatrix}.$$

The adjoint operator has the representation

$$\begin{aligned}(T_*(z)^*\xi)(x) = & \frac{1}{W(\overline{z})}\{-\alpha_b v_a(x,\overline{z})\xi^b \\ & + \alpha_N(v_b(x_N,\overline{z})v_a(x,\overline{z})\chi_{[a,x_N)}(x) + v_a(x_N,\overline{z})v_b(x,\overline{z})\chi_{[x_N,b]})\xi^N \\ & \vdots \\ & + \alpha_1(v_b(x_1,\overline{z})v_a(x,\overline{z})\chi_{[a,x_1)}(x) + v_a(x_1,\overline{z})v_b(x,\overline{z})\chi_{[x_1,b]})\xi^1 \\ & + \alpha_a v_b(x,\overline{z})\xi^a\},\end{aligned}$$

for $x \in [a,b]$.

Let us collect some properties of the above operators.

Lemma 3.1 *Let $V \in \mathsf{L}^2(a,b)$ be real-valued, and $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$. Then we have*

$$(H^* - z)^{-1} - (H - z)^{-1} = -iT_*(\overline{z})^*T_*(z) = -iT(\overline{z})^*T(z), \tag{3.3}$$

for $z \in \varrho(H) \cap \varrho(H^*)$.

Proof. A straightforward calculation shows that

$$(H^*f,g) - (f,H^*g) = i\sum_{j=0}^{N+1} \alpha_i^2 f(x_j)\overline{g(x_j)},$$

for $f, g \in \mathsf{D}(H^*)$. Setting $f = (H^* - z)^{-1}h$ and $g = (H^* - \overline{z})^{-1}k$ with $h, k \in \mathcal{H}$, $z, \overline{z} \in \varrho(H^*)$, we obtain

$$((H^* - z)^{-1}h, k) - (h, (H^* - \overline{z})^{-1}k) = -i\langle T_*(z)h, T_*(\overline{z})k\rangle_{\mathbb{C}^{N+2}},$$

and the first equality in (3.3) is proven. The second relation can be proven in the same fashion. □

The characteristic function $\Theta_H(\cdot)$ is a crucial element in the study of completely non-selfadjoint operators. It is a purely contractive valued and analytic function on $\overline{\mathbb{C}_-}$, where $\mathbb{C}_- := \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) < 0\}$, cf. [FN70]. The characteristic function $\Theta_H(\cdot)$ of the maximal dissipative operator H is a $(N+2) \times (N+2)$ matrix-valued function satisfying the relation

$$\Theta_H(z)T(z)f = T_*(z)f, \quad z \in \varrho(H) \cap \varrho(H^*), \quad f \in \mathcal{H}. \tag{3.4}$$

Let us compute the characteristic function $\Theta_H(\cdot)$ of H:

Theorem 3.2 *Let $V \in \mathsf{L}^2(a,b)$ be real-valued and $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_-$. Then the characteristic function of H is given by*

$$\Theta_H(z) = I_{\mathbb{C}^{N+2}} - \frac{i}{W_*(z)}\times$$

$$\begin{pmatrix} -\alpha_b^2 v_{*a}(b,z) & \alpha_b\alpha_N v_{*a}(x_N,z) & \cdots & \alpha_b\alpha_1 v_{*a}(x_1,z) & \alpha_b\alpha_a \\ \alpha_N\alpha_b v_{*a}(x_N,z) & -\alpha_N^2 v_{*a}(x_N,z)v_{*b}(x_N,z) & \cdots & -\alpha_N\alpha_1 v_{*a}(x_1,z)v_{*b}(x_N,z) & -\alpha_N\alpha_a v_{*b}(x_N,z) \\ \vdots & \vdots & & \vdots & \vdots \\ \alpha_1\alpha_b v_{*a}(x_1,z) & -\alpha_1\alpha_N v_{*a}(x_1,z)v_{*b}(x_N,z) & \cdots & -\alpha_1^2 v_{*a}(x_1,z)v_{*b}(x_1,z) & -\alpha_1\alpha_a v_{*b}(x_1,z) \\ \alpha_a\alpha_b & -\alpha_a\alpha_N v_{*b}(x_N,z) & \cdots & -\alpha_a\alpha_1 v_{*b}(x_1,z) & -\alpha_a^2 v_{*b}(a,z) \end{pmatrix} \tag{3.5}$$

for $z \in \varrho(H) \cap \varrho(H^*)$.

Proof. It remains to verify that $\Theta_H(\cdot)$ given by (3.5) satisfies (3.4).

One easily checks, that equation (3.5) can be written as

$$\Theta_H(z) = I_{\mathbb{C}^{N+2}} - i\alpha T(\overline{z})^*. \tag{3.6}$$

Using equation (3.3) we get

$$\Theta_H(z)T(z) = T(z) - i\alpha T(\overline{z})^* T(z) = \alpha(H^* - z)^{-1} = T_*(z).$$

Thus equation (3.4) is verified. $\square$

Since

$$T(z)^*T(z) - T_*(z)^*T_*(z) = -2\mathrm{Im}(z)T(z)^*T(\overline{z})T(\overline{z})^*T(z), \quad \text{for } z \in \varrho(H) \cap \varrho(H^*),$$

we have for $z \in \mathbb{C}_- \cap \varrho(H)$ that

$$\|\Theta_H(z)T(z)f\|^2 = \|T_*(z)f\|^2 \leq \|T(z)f\|^2, \quad f \in \mathcal{H}.$$

Thus $\Theta_H(z)$ is a contraction for $z \in \mathbb{C}_- \cap \varrho(H)$. Since the spectrum of H consists of only isolated eigenvalues in $\mathbb{C}_-$, we get that the characteristic function $\Theta_H(z)$ admits a unique continuation to all $z \in \overline{\mathbb{C}_-}$, cf. (3.6).

4 Dilations

Since H is a maximal dissipative operator, there exists a larger Hilbert space $\mathcal{K}$ containing $\mathcal{H}$, i.e. $\mathcal{H} \subseteq \mathcal{K}$, and a selfadjoint operator K on $\mathcal{K}$ such that

$$P^{\mathcal{K}}_{\mathcal{H}}(K - z)^{-1}_{\restriction \mathcal{H}} = (H - z)^{-1}, \quad z \in \mathbb{C}_+, \tag{4.1}$$

(see [FN70]). The operator K is called a dilation of H. K is said to be a minimal selfadjoint dilation, if

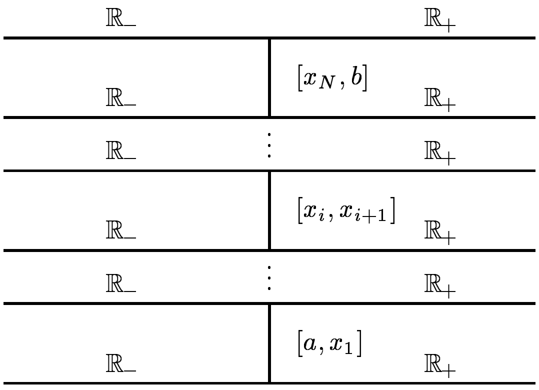
$$\operatorname*{clospan}_{z \in \mathbb{C}\setminus\mathbb{R}} (K - z)^{-1}\mathcal{H} = \mathcal{K}. \tag{4.2}$$

All minimal selfadjoint dilation of a maximal dissipative operator are isomorphic. In particular, all minimal selfadjoint dilation are unitarily equivalent.

The next step in our investigations is to obtain an explicit description of the selfadjoint dilation of H. Let us introduce the Hilbert space $\mathcal{K}$ defined by

$$\mathcal{K} := \mathcal{D}_- \oplus \mathcal{H} \oplus \mathcal{D}_+,$$

with $\mathcal{D}_\pm := \mathsf{L}^2(\mathbb{R}_\pm, \mathbb{C}^{N+2})$. Introducing the domain $\hat{\Omega}$



we get $\mathcal{K} = \mathsf{L}^2(\hat{\Omega}, dx)$. For $\vec{g} \in \mathcal{K}$ we write

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

where

$$g_- = \begin{pmatrix} g^b_-(x) \\ g^N_-(x) \\ \vdots \\ g^1_-(x) \\ g^a_-(x) \end{pmatrix} \quad \text{and} \quad g_+ = \begin{pmatrix} g^b_+(x) \\ g^N_+(x) \\ \vdots \\ g^1_+(x) \\ g^a_+(x) \end{pmatrix},$$

for $x \in \mathbb{R}_-$ and $x \in \mathbb{R}_+$, respectively. Furthermore we will need the $(N+2) \times (N+2)$-matrices $K^b_\pm$, $K^a_\pm$, and $K^j_\pm$, $j = 1, \cdots, N$, defined by

$$K^b_- := \frac{1}{\alpha_b} \begin{pmatrix} 1 & 0 & \cdots & 0 & -\kappa_b \\ 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \end{pmatrix}, \quad K^a_- := \frac{1}{\alpha_a} \begin{pmatrix} 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \\ 1 & 0 & \cdots & 0 & \kappa_a \end{pmatrix},$$

$$K^j_- := \frac{1}{\alpha_j} \begin{pmatrix} 0 & & \cdots & & 0 \\ \vdots & & & & \vdots \\ 1 & 0 & \cdots & 0 & \kappa_j \\ \vdots & & & & \vdots \\ 0 & & \cdots & & 0 \end{pmatrix} \leftarrow (j+1)\text{-th row},$$

and $K^b_+ := \overline{K^b_-}$, $K^a_+ := \overline{K^a_-}$, $K^j_+ := \overline{K^j_-}$, as well as

$$E = \begin{pmatrix} 0 & \cdots & \cdots & 0 & 1 \\ 0 & \cdots & \cdots & 0 & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & \cdots & \cdots & 0 \\ -1 & 0 & \cdots & \cdots & 0 \end{pmatrix}.$$

We set

$$g_a = \begin{pmatrix} \frac{1}{2m(a)} g'(a) \\ 0 \\ \vdots \\ 0 \\ g(a) \end{pmatrix}, \quad g_b = \begin{pmatrix} \frac{1}{2m(b)} g'(b) \\ 0 \\ \vdots \\ 0 \\ g(b) \end{pmatrix}, \quad \text{and} \quad g_j = \begin{pmatrix} \Delta(g)(x_j) \\ 0 \\ \vdots \\ 0 \\ g(x_j) \end{pmatrix}.$$

Theorem 4.1 *Let* $V \in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V) = 0$, $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$, *and* $x_1, \cdots, x_N \in (a,b)$, *such that* $x_1 < x_2 < \cdots < x_N$. *Then the operator* K *defined by*

$$\mathsf{D}(K) := \left\{ \vec{g} \in \mathcal{K} \;\middle|\; \begin{array}{l} g_\pm \in \mathsf{W}^{1,2}(\mathbb{R}_\pm, \mathbb{C}^{N+2}), g \in \mathsf{W}^{1,2}(a,b), \\ \frac{1}{m} g' \in \mathsf{W}^{1,2}(a, x_1) \oplus \bigoplus_{j=1}^N \mathsf{W}^{1,2}(x_j, x_{j+1}) \oplus \mathsf{W}^{1,2}(x_N, b) \\ K^a_- g_a + \sum_{j=1}^N K^j_- g_j + K^b_- g_b = g_-(0), \\ K^a_+ g_a + \sum_{j=1}^N K^j_+ g_j + K^b_+ g_b = g_+(0) \end{array} \right\} \tag{4.3}$$

and

$$K\vec{g} := -i\frac{d}{dx} g_- \oplus l(g) \oplus -i\frac{d}{dx} g_+, \qquad \vec{g} \in \mathsf{D}(K),$$

is selfadjoint.

The proof is essentially the same as in [KNR01b], so we omit it.

Figure 1 shows the boundary conditions of the operator K with respect to the domain $\hat{\Omega}$.

To show that K is the minimal dilation corresponding to H, let us compute the resolvent of K.

Theorem 4.2 *Assume that* $V \in \mathsf{L}^2(a,b)$ *is real-valued and* $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$. *Then the resolvent of* K *admits the representation*

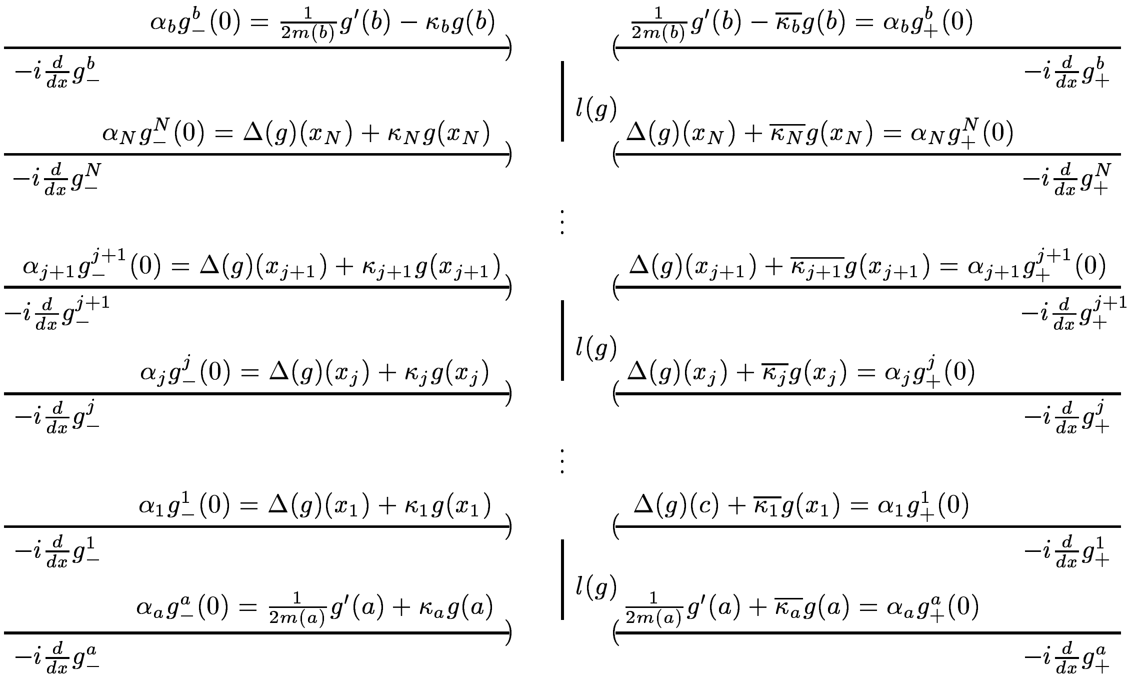
$$\begin{aligned}
&(K-z)^{-1}(f_- \oplus f \oplus f_+)(x) \qquad (4.4)\\
&\quad = i\int_{-\infty}^{x} e^{i(x-y)z} f_-(y)\,dy \oplus ((H-z)^{-1}f)(x) + i\left(T_*(\overline{z})^* \int_{-\infty}^{0} e^{-iyz} f_-(y)\,dy\right)(x)\\
&\quad\quad \oplus\, i\int_{0}^{x} e^{i(x-y)z} f_+(y)\,dy + ie^{izx}T(z)f + i\Theta_H(\overline{z})^* \int_{-\infty}^{0} e^{i(x-y)z} f_-(y)\,dy,
\end{aligned}$$

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

$$\begin{aligned}
&(K-z)^{-1}(f_- \oplus f \oplus f_+)(x) \qquad (4.5)\\
&\quad = -i\int_{x}^{0} e^{i(x-y)z} f_-(y)\,dy - ie^{izx}T_*(z)f - i\Theta_H(z)\int_{0}^{\infty} e^{i(x-y)z} f_+(y)\,dy\\
&\quad\quad \oplus ((H^*-z)^{-1}f)(x) - i\left(T(\overline{z})^* \int_{0}^{\infty} e^{-iyz} f_+(y)\,dy\right)(x) \oplus -i\int_{x}^{\infty} e^{i(x-y)z} f_+(y)\,dy,
\end{aligned}$$

for $\mathrm{Im}(z) < 0$, *where* $\vec{f} = f_- \oplus f \oplus f_+ \in \mathcal{K}$.

Figure 1: Boundary conditions of the dilation K



Proof. We will only prove equation (4.4) since the equality of (4.5) can be shown in the same fashion. Let $\mathrm{Im}(z) > 0$, $\vec{f} \in \mathcal{K}$. We set

$$\begin{aligned} g_-(x) &:= i \int_{-\infty}^{x} e^{i(x-y)z} f_-(y)\,dy, \\ g(x) &:= ((H-z)^{-1} f)(x) + i \left(T_*(\overline{z})^* \int_{-\infty}^{0} e^{-iyz} f_-(y)\,dy \right)(x) \\ g_+(x) &:= i \int_0^x e^{i(x-y)z} f_+(y)\,dy + i e^{izx} T(z) f + i \Theta_H(\overline{z})^* \int_{-\infty}^{0} e^{i(x-y)z} f_-(y)\,dy. \end{aligned} \tag{4.6}$$

One easily verifies that

$$(K - z)(g_- \oplus g \oplus g_+) = f_- \oplus f \oplus f_+.$$

Thus it remains to show that $\vec{g}$ satisfies the boundary conditions (4.3). We set $h = (H-z)^{-1} f$ and get

$$g_a = h_a + G_a g_-(0), \quad g_j = h_j + G_j g_-(0), \quad g_b = h_b + G_b g_-(0), \quad \forall j = 1, \cdots, N, \tag{4.7}$$

where

$$G_a := \begin{pmatrix} -\kappa_a (T_*(\overline{z})^* e_b)(a) & \cdots & -\kappa_a (T_*(\overline{z})^* e_1)(a) & \frac{1}{2m(a)} (T_*(\overline{z})^* e_a)'(a) \\ 0 & \cdots & 0 & 0 \\ \vdots & & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \\ (T_*(\overline{z})^* e_b)(a) & \cdots & (T_*(\overline{z})^* e_1)(a) & (T_*(\overline{z})^* e_a)(a) \end{pmatrix},$$

$$G_b := \begin{pmatrix} \frac{1}{2m(b)} (T_*(\overline{z})^* e_b)'(b) & \kappa_b (T_*(\overline{z})^* e_N)(b) & \cdots & \kappa_b (T_*(\overline{z})^* e_a)(b) \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \\ (T_*(\overline{z})^* e_b)(b) & (T_*(\overline{z})^* e_N)(b) & \cdots & (T_*(\overline{z})^* e_a)(b) \end{pmatrix},$$

and

$$G_j := \begin{pmatrix} -\kappa_j (T_*(\overline{z})^* e_b)(x_j) & \cdots & \Delta (T_*(\overline{z})^* e_j)(x_j) & \cdots & -\kappa_j (T^*(\overline{z})^* e_a)(x_j) \\ 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \\ (T_*(\overline{z})^* e_b)(x_j) & \cdots & (T_*(\overline{z})^* e_j)(x_j) & \cdots & (T^*(\overline{z})^* e_a)(x_j) \end{pmatrix},$$

where $e_a, e_j, e_b \in \mathbb{C}^{N+2}$ are given by

$$e_b = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad e_a = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad e_j = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}.$$

Since $h \in \mathsf{D}(H)$,

$$K_-^a h_a = K_-^j h_j = K_-^b h_b = 0, \quad \forall j = 1, \cdots, N. \tag{4.8}$$

A straightforward calculation shows, that

$$K_-^a G_a \xi = \xi^a e_a, \quad K_-^b G_b \xi = \xi^b e_b, \quad K_-^j G_j \xi = \xi^j e_j, \quad \forall j = 1, \cdots, N,$$

where $\xi \in \mathbb{C}^{N+2}$ (see (3.2)). Therefore we get by (4.7) and (4.8)

$$K_-^a g_a + \sum_{j=1}^{N} K_-^j g_j + K_-^b g_b = g_-(0).$$

Using (4.6) we get

$$g_+(0) = iT(z)f + \Theta_H(\overline{z})^* g_-(0).$$

Since

$$K_+^a h_a = -i\alpha_a h(a) e_a, \quad K_+^b h_b = i\alpha_b h(b) e_b, \quad K_+^j h_j = -i\alpha_j h(x_j) e_j,\ \forall j = 1, \cdots, N,$$

we find by equation (3.1)

$$K_+^a h_a + \sum_{j=1}^{N} K_+^j h_j + K_+^b h_b = iT(z)f.$$

Note that

$$\Theta_H(\overline{z})^* = 1 + i\alpha T_*(\overline{z})^*. \tag{4.9}$$

We have

$$\begin{aligned} K_+^a G_a &= \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \\ -i\alpha_a (T_*(\overline{z})^* e_b)(a) & \cdots & 1 - i\alpha_a (T_*(\overline{z})^* e_a)(a) \end{pmatrix} \\ &= \begin{pmatrix} 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \\ i\langle \alpha T_*(\overline{z})^* e_b, e_a \rangle_{\mathbb{C}^{N+2}} & \cdots & 1 + i\langle \alpha T_*(\overline{z})^* e_a, e_a \rangle_{\mathbb{C}^{N+2}} \end{pmatrix}, \end{aligned}$$

and similar

$$K_+^b G_b = \begin{pmatrix} 1 + i\langle \alpha T_*(\overline{z})^* e_b, e_b \rangle_{\mathbb{C}^{N+2}} & \cdots & i\langle \alpha T_*(\overline{z})^* e_a, e_b \rangle_{\mathbb{C}^{N+2}} \\ 0 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 0 \end{pmatrix},$$

$$K_+^j G_j = \begin{pmatrix} 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \\ i\langle \alpha T_*(\overline{z})^* e_b, e_j \rangle_{\mathbb{C}^{N+2}} & \cdots & 1 + i\langle \alpha T_*(\overline{z})^* e_j, e_j \rangle_{\mathbb{C}^{N+2}} & \cdots & i\langle \alpha T_*(\overline{z})^* e_a, e_j \rangle_{\mathbb{C}^{N+2}} \\ 0 & \cdots & 0 & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & 0 & \cdots & 0 \end{pmatrix},$$

for all $j = 1, \cdots, N$. Hence we get by (4.9)

$$K_+^a G_a + \sum_{j=1}^{N} K_+ G_j + K_+ G_b = \Theta_H(\overline{z})^*$$

and finally

$$K_+ g_a + \sum_{j=1}^{N} K_+ g_j + K_+^b g_b = g_+(0)$$

which completes the proof. □

Using the expressions (4.4) and (4.5) for the resolvent of K, one easily verifies (4.1) and (4.2).

5 Eigenfunction expansion

The selfadjoint operator K is absolutely continuous and $\sigma(K) = \sigma_{ac}(K) = \mathbb{R}$, i.e. the spectrum of K coincides with the real line. Its multiplicity is $N+2$. We are now going to compute the generalized eigenfunction $\vec{\phi}(\cdot,\lambda)$, $\lambda \in \mathbb{R}$, of K. We set

$$\vec{\phi}(x,\lambda) = \phi_-(x,\lambda) \oplus \phi(x,\lambda) \oplus \phi_+(x,\lambda),$$

for $x \in \hat{\Omega}$, where

$$\phi_-(x,\lambda) = \begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_-, \quad \phi_+(x,\lambda) = \begin{pmatrix} \phi_+^b(x,\lambda) \\ \phi_+^N(x,\lambda) \\ \vdots \\ \phi_+^1(x,\lambda) \\ \phi_+^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_+.$$

From

$$\begin{aligned} (K\vec{\phi})(x,\lambda) &= -i\frac{d}{dx}\phi_-(x,\lambda) \oplus l(\phi(\cdot,\lambda))(x) \oplus -i\frac{d}{dx}\phi_+(x,\lambda) \\ &= \lambda(\phi_-(x,\lambda) \oplus \phi(x,\lambda) \oplus \phi_+(x,\lambda)), \end{aligned}$$

$x \in \hat{\Omega}$, we find the equations

$$-i\frac{d}{dx}\begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix} = \lambda \begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_-, \tag{5.1}$$

$$l(\phi(\cdot,\lambda))(x) = \lambda\phi(x,\lambda), \quad x \in [a,b], \tag{5.2}$$

and

$$-i\frac{d}{dx}\begin{pmatrix} \phi_+^b(x,\lambda) \\ \phi_+^N(x,\lambda) \\ \vdots \\ \phi_+^1(x,\lambda) \\ \phi_+^a(x,\lambda) \end{pmatrix} = \lambda \begin{pmatrix} \phi_-^b(x,\lambda) \\ \phi_-^N(x,\lambda) \\ \vdots \\ \phi_-^1(x,\lambda) \\ \phi_-^a(x,\lambda) \end{pmatrix}, \quad x \in \mathbb{R}_+. \tag{5.3}$$

The equation (5.1) and (5.3) have the solutions

$$\phi_-(x,\lambda) = C_-e^{ix\lambda}, \quad C_- \in \mathbb{C}^{N+2},\ x \in \mathbb{R}_-,$$

and

$$\phi_+(x,\lambda) = C_+e^{ix\lambda}, \quad C_+ \in \mathbb{C}^{N+2},\ x \in \mathbb{R}_+.$$

The solution of (5.2) is given by a linear combination of the elementary solutions $v_a(x,\lambda)$ and $v_b(x,\lambda)$ on each interval $[x_j, x_{j+1})$, i.e.

$$\phi(x,\lambda) = \sum_{j=0}^{N} \left(c_a^j v_a(x,\lambda) + c_b^j v_b(x,\lambda), \right) \chi_{[x_j,x_{j+1})}(x). \tag{5.4}$$

The eigenfunctions have to satisfy the boundary conditions, i.e.

$$K_-^a\phi_a(\lambda) + \sum_{j=1}^{N} K_-^j\phi_j(\lambda) + K_-^b\phi_b(\lambda) = \phi_-(0,\lambda). \tag{5.5}$$

and

$$K_+^a\phi_a(\lambda) + \sum_{j=1}^{N} K_+^j\phi_j(\lambda) + K_+^b\phi_b(\lambda) = \phi_+(0,\lambda). \tag{5.6}$$

Furthermore the condition

$$(c_a^{j+1} - c_a^j)v_a(x_j,\lambda) + (c_b^{j+1} - c_b^j)v_b(x_j,\lambda) = 0, \quad \forall j = 0,\cdots,N+1,$$

has to be satisfied. A straightforward calculation shows that

$$c_a^{N+1} = -\frac{\alpha_b}{W(z)},C_-^b, \quad c_a^j = c_a^{j+1} + \frac{\alpha_j v_b(x_j,\lambda)}{W(\lambda)}C_-^j, \quad j = 0,\cdots,N, \tag{5.7}$$

as well as

$$c_b^0 = \frac{\alpha_a}{W(z)}C_-^a, \quad c_b^j = c_b^{j+1} - \frac{\alpha_j v_a(x_j,\lambda)}{W(\lambda)}C_-^j, \quad j = 1,\cdots,N+1. \tag{5.8}$$

Inserting equations (5.7) and (5.8) in (5.4) finally yields

$$\phi(x,\lambda) = (T_*(\lambda)^*C_-)(x). \tag{5.9}$$

By inserting (5.9) in (5.6) we find

$$C_+ = \Theta_H(\lambda)^*C_-, \quad \lambda \in \mathbb{R}.$$

Therefore we get

$$\vec{\phi}^{C_-}(x,\lambda) := e^{ix\lambda}C_- \oplus (T_*(\lambda)^*C_-)(x) \oplus e^{ix\lambda}\Theta_H(\lambda)^*C_-,$$

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

A calculation as in [KNR01b] shows that

$$\left(\frac{1}{\sqrt{2\pi}}\vec{\phi}^{C_-}(\cdot,\lambda), \frac{1}{\sqrt{2\pi}}\vec{\phi}^{C'_-}(\cdot,\lambda')\right)_{\mathcal{K}} = \delta(\lambda-\lambda')\langle C_-, C'_-\rangle.$$

Introducing the notions

$$\vec{\phi}(\cdot,\lambda,j) := \frac{1}{\sqrt{2\pi}}\vec{\phi}^{e_j}(\cdot,\lambda), \quad j = 0,\cdots,N+1, \tag{5.10}$$

where we have set $e_a = e_0$ and $e_b = e_{N+1}$, we get the following theorem.

Theorem 5.1 *Assume* $V \in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V) = 0$, *and* $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$. *Then the functions*

$$\{\vec{\phi}(\cdot,\lambda,a), \vec{\phi}(\cdot,\lambda,1), \cdots, \vec{\phi}(\cdot,\lambda,N), \vec{\phi}(\cdot,\lambda,b)\}_{\lambda\in\mathbb{R}}$$

perform a complete orthonormal system of generalized eigenfunctions of K, *i.e.*

$$\left(\vec{\phi}(\cdot,\lambda,\tau), \vec{\phi}(\cdot,\lambda',\tau')\right)_{\mathcal{K}} = \delta(\lambda-\lambda')\delta_{\tau\tau'}, \quad \lambda,\lambda' \in \mathbb{R}, \quad \tau,\tau' = a,1,\cdots,N,b,$$

and their linear span, i.e. elements of the form

$$f(x) = \int_{\mathbb{R}} \sum_{\tau=a,1,\cdots,N,b} \vec{\phi}(\cdot,\lambda,\tau)g^\tau(\lambda)\,d\lambda,$$

where g^τ ,$\tau = a,1,\cdots,N,b$, *are smooth functions with compact support, is dense in* $\mathcal{K}$.

We say that $\{e^a(\lambda), e^1(\lambda), \cdots, e^N(\lambda), e^b(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of orthogonal bases in $\mathbb{C}^{N+2}$, if the components of the vectors $e^\tau(\lambda)$, $\tau = a,1,\cdots,N,b$, are Lebesgue measurable functions such that $\langle e^\tau(\lambda), e^\xi(\lambda)\rangle = \delta_{\tau,\xi}$ for a.e. $\lambda \in \mathbb{R}$. Thus we get

Corollary 5.2 *Suppose that* $V \in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V) = 0$, $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$, *and* $x_1, \cdots, x_N \in (a,b)$ *with* $x_1 < x_2 < \cdots < x_N$. *If* $\{e^a(\lambda), e^1(\lambda), \cdots, e^N(\lambda), e^b(\lambda)\}_{\lambda\in\mathbb{R}}$ *is a measurable family of orthogonal bases in* $\mathbb{C}^{N+2}$, *then the system of eigenfunctions*

$$\{\vec{\phi}(\cdot,\lambda,e^a(\lambda)), \vec{\phi}(\cdot,\lambda,e^1(\lambda)), \cdots, \vec{\phi}(\cdot,\lambda,e^N(\lambda)), \vec{\phi}(\cdot,\lambda,e^b(\lambda))\}_{\lambda\in\mathbb{R}},$$

where

$$\vec{\phi}(\cdot,\lambda,e^\tau(\lambda)) := \frac{1}{\sqrt{2\pi}}\vec{\phi}^{e^j(\lambda)}(\cdot,\lambda), \quad \tau = a, \cdots, b,$$

performs a complete orthonormal system of generalized eigenfunctions of K.

The generalized eigenfunctions $\phi(\cdot,\lambda,\tau)$ are usually called the incoming eigenfunctions. By the use of the incoming eigenfunctions, one defines a transform $\mathcal{F} : \mathcal{K} \to \hat{\mathcal{K}} := \mathsf{L}^2(\mathbb{R}, \mathbb{C}^{N+2})$ by

$$(\mathcal{F}\vec{g})(\lambda) =: \hat{g}(\lambda) = \begin{pmatrix} \hat{g}^b(\lambda) \\ \hat{g}^N(\lambda) \\ \vdots \\ \hat{g}^1(\lambda) \\ \hat{g}^a(\lambda) \end{pmatrix},$$

where

$$\hat{g}^\tau(\lambda) := \int_{\hat{\Omega}} \Big(\vec{g}(x), \vec{\phi}(x,\lambda,\tau)\Big)_{\mathcal{K}}\, dx.$$

$\mathcal{F}$ is a unitary operator and called the incoming Fourier transform. The inverse incoming Fourier transform $\mathcal{F}^{-1}$ is given by

$$\left(\mathcal{F}^{-1}\hat{g}\right)(x) = \int_{\mathbb{R}} \sum_{\tau=a,1,\cdots,N,b} \vec{\phi}(\cdot,\lambda,\tau)\hat{g}^\tau(\lambda)\, d\lambda, \quad \hat{g} \in \hat{\mathcal{K}}.$$

We note that

$$\mathcal{F}K\mathcal{F}^{-1} = M, \tag{5.11}$$

where M is the multiplication operator on $\hat{\mathcal{K}}$ given by

$$\begin{aligned} \mathsf{D}(M) &:= \{\hat{g} \in \hat{\mathcal{K}} \,|\, \lambda\hat{g}(\lambda) \in \hat{\mathcal{K}}\}, \\ (M\hat{g})(\lambda) &:= \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathsf{D}(M). \end{aligned}$$

6 Carrier density

According to [KNR01c] we call $\varrho : \mathcal{K} \to \mathcal{K}$ a density matrix, if ϱ is a bounded, non-negative operator. A density matrix ϱ is called a steady state, if it commutes with K. For steady states ϱ there exists a function $\varrho(\cdot) \in \mathsf{L}^\infty(\mathbb{R}, \mathfrak{B}(\mathbb{C}^{N+2}))$ such that the multiplication operator $\hat{\varrho}$ defined by

$$\begin{aligned} \mathsf{D}(\hat{\varrho}) &:= \{\hat{g} \in \mathcal{K} \,|\, \varrho(\lambda)\hat{g}(\lambda) \in \mathcal{K}\}, \\ (\hat{\varrho}\hat{g})(\lambda) &:= \varrho(\lambda)\hat{g}(\lambda), \quad \hat{g} \in \mathsf{D}(\hat{\varrho}), \end{aligned}$$

is unitarily equivalent to ϱ, i.e.

$$\varrho = \mathcal{F}^{-1}\hat{\varrho}\mathcal{F}.$$

Since $\varrho \geq 0$ we get $\varrho(\lambda) \geq 0$ for a.e. $\lambda \in \mathbb{R}$.

The time evolution of a given density matrix ϱ is given by

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

cf. [LL71]. If ϱ commutes with K, we have $\varrho(t) = \varrho$ for all $t \in \mathbb{R}$. This justifies the definition of steady states.

Definition 6.1 A bounded selfadjoint operator A on a Hilbert space $\mathcal{K}$ is called an observable. We say that the observable A

1. is admissible with respect to ϱ if ϱA is a trace class operator, i.e $\varrho A \in \mathfrak{B}_1(\mathcal{K})$,
2. is admissible with respect to K if $E_K(\Delta)A \in \mathfrak{B}_1(\mathcal{K})$ for each bounded interval $\Delta \subset \mathbb{R}$, where $E_K(\Delta)$ denotes the spectral projection of K on Δ.

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

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

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

$$(U(\omega)\vec{f})(x) = 0 \oplus \chi_\omega(x) f(x) \oplus 0, \quad \vec{f} = f_- \oplus f \oplus f_+ \in \mathcal{K},$$

for any Borel subset $\omega \subseteq [a,b]$. We remark that $U(\omega)$ is a projection on $\mathcal{K}$ with $\mathrm{ran}(U(\omega)) \subseteq \mathcal{H}$.

Let us introduce some more notions: We set

$$\Phi(x,\lambda) = \begin{pmatrix} \phi(x,\lambda,N+1) \\ \vdots \\ \phi(x,\lambda,0) \end{pmatrix},$$

and $\overline{\Phi(x,\lambda)}$ denotes the the vector $\Phi(x,\lambda)$ with each element complex conjugated.

As in [KNR01c] one proves the following lemma:

Lemma 6.2 *Assume that* $m + \frac{1}{m} \in \mathsf{L}^\infty(a,b)$, $V \in \mathsf{L}^2(a,b)$, $\mathrm{Im}(V) = 0$, $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$, *and* $x_1, \cdots, x_n \in (a,b)$ *such that* $x_1 < x_2 < \cdots < x_N$.

1. *The observable* $U(\omega)$ *is admissible with respect to the minimal selfadjoint dilation* K *of the maximal dissipative operator* H *for any Borel set* $\omega \subseteq [a,b]$. *Furthermore, we get the representation*

$$\mathrm{tr}(\varrho U(\omega) E_K(\Delta)) = \int_\Delta \mathrm{tr}(\varrho(\lambda) U(\omega)(\lambda))\, d\lambda,$$

for any bounded Borel set $\Delta \subset \mathbb{R}$ *and any steady state* ϱ, *where*

$$U(\omega)(\lambda) := \int_\omega D(x,\lambda)\, dx,$$

with

$$D(x,\lambda) := \overline{\Phi(x,\lambda)}\, \Phi(x,\lambda)^T$$

2. *If the steady state* ϱ *satisfies the condition*

$$C_{\hat{\varrho}} := \sup_{\lambda \in \mathbb{R}} \sqrt{\lambda^2 + 1} \|\varrho(\lambda)\|_{\mathfrak{B}(\mathbb{C}^{N+2})} < \infty, \tag{6.1}$$

then the observable $U(\omega)$ *is admissible with respect to* ϱ *for any Borel set* $\omega \subseteq [a,b]$. *Furthermore we have*

$$\mathrm{tr}(\varrho U(\omega)) = \int_\mathbb{R} \mathrm{tr}(\varrho(\lambda) U(\omega)(\lambda))\, d\lambda.$$

We set

$$u_\varrho(x,\lambda) := \operatorname{tr}(\varrho(\lambda)D(x,\lambda)),$$

for $x \in [a,b]$ and $\lambda \in \mathbb{R}$. Note that

$$u_\varrho(x,\lambda) = \left\langle \varrho(\lambda)^T \Phi(x,\lambda), \Phi(x,\lambda) \right\rangle, \tag{6.2}$$

where $\varrho(\lambda)^T$ denotes the transposed matrix of $\varrho(\lambda)$. Since $\varrho(\lambda)$ is non-negative, we get by the representation (6.2) that $u_\varrho(x,\lambda) \geq 0$ for $x \in [a,b]$ and a.e. $\lambda \in \mathbb{R}$. If the condition (6.1) is satisfied, we get by Lemma 6.2

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

for any Borel set $\omega \subseteq [a,b]$. Hence by Fubini's Theorem we get

$$\mathbb{E}_\varrho(U(\omega)) = \int_\omega u_\varrho(x)\,dx, \tag{6.3}$$

where

$$u_\varrho(x) := \int_{\mathbb{R}} u_\varrho(x,\lambda)\,d\lambda \geq 0, \quad x \in [a,b], \tag{6.4}$$

thus $u_\varrho \in \mathsf{L}^1(a,b)$. Clearly $\mathbb{E}_\varrho(U(\cdot))$ defines a measure which is absolutely continuous with respect to the Lebesgue measure. Since $\mathbb{E}_\varrho(U(\omega))$ can be interpreted as the number of carriers in $\omega \subseteq [a,b]$, its Radon-Nikodym derivative can be viewed as the carrier density of the system described by K. Since K is the dilation corresponding to the maximal dissipative operator H and $U(\omega)$ acts only on $\mathcal{H}$, we identify u_ϱ with the carrier density of the system described by H.

Note that

$$u_\varrho(x,\lambda) = \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)), \tag{6.5}$$

for $x \in [a,b]$ and $\lambda \in \mathbb{R}$. We call the matrix $D(x,\lambda)$ the carrier density observable and $u_\varrho(x,\lambda)$ the carrier density of the system described by H at point $x \in [a,b]$ and energy $\lambda \in \mathbb{R}$. This is justified since (6.5) can be seen as expectation value of the carrier density observable.

Furthermore we have

$$u_\varrho(x) = \int_{\mathbb{R}} \mathbb{E}_{\varrho(\lambda)}(D(x,\lambda)), \quad x \in [a,b],$$

i.e. the carrier density for each point x is the sum of the expectation values of the carrier density observable for the point x over all energies.

For real-valued $h \in \mathsf{L}^\infty(a,b)$ we define the multiplication operator $M(h)$ on the Hilbert space $\mathcal{K}$ by

$$(M(h)\vec{f})(x) = 0 \oplus h(x)f(x) \oplus 0, \quad \vec{f} = f_- \oplus f \oplus f_+ \in \mathcal{K}.$$

We note that $M(\chi_\omega) = U(\omega)$, in particular $M(\chi_\Omega) = U(\Omega) = P^{\mathcal{K}}_{\mathcal{H}}$. Since

$$\varrho M(h) = \varrho U(\Omega) M(h), \qquad h \in \mathsf{L}^\infty(a,b),$$

we get that the observable $M(h)$ is admissible with respect to ϱ.

Lemma 6.3 *Assume that* $m + \frac{1}{m} \in \mathsf{L}^\infty$, $V \in \mathsf{L}^2(a,b)$ *real-valued, and* $\kappa_a, \kappa_1 \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$. *If the steady state* ϱ *satisfies the condition* (6.1), *then the carrier density* u_ϱ *defined by* (6.4) *is a non-negative* L^1*-function such that*

$$\operatorname{tr}(\varrho M(h)) = \int_a^b u_\varrho(x)h(x)\,dx, \tag{6.6}$$

for any real-valued function $h \in \mathsf{L}^\infty([a,b])$. *In particular one has*

$$\|u_\varrho\|_{\mathsf{L}^1(\omega)} = \operatorname{tr}(\varrho U(\omega)) \leq C_{\hat{\varrho}} \|(K-i)^{-1} P^{\mathcal{K}}_{\mathcal{H}}\|_{\mathfrak{B}_1} \tag{6.7}$$

for each Borel set $\omega \subseteq [a,b]$.

Proof. By (6.3) we get that (6.6) holds for $h = \chi_\Omega$. By linearity (6.6) can be extended for arbitrary step functions h. Since u_ϱ is from $\mathsf{L}^1(a,b)$ and $\varrho U(\Omega)$ is of trace class, (6.6) admits a continuation to all L^∞-functions h, which proves the first part of the lemma.

Since $(K-i)^{-1}P^{\mathcal{K}}_{\mathcal{H}}$ is a trace class operator and since $\varrho(K-i)$ is a bounded operator whose norm can be estimated by $C_{\hat{\varrho}}$, we obtain

$$\operatorname{tr}(\varrho(K-i)(K-i)^{-1}U(\omega)) \le C_{\hat{\varrho}} \|(K-i)^{-1}P^{\mathcal{H}}_{\mathcal{K}}\|_{\mathfrak{B}_1}.$$

This verifies (6.7). □

Suppose that $\{\varrho(\lambda)\}_{\lambda\in\mathbb{R}}$ is a measurable family of non-negative selfadjoint operators on $\mathbb{C}^{N+2}$. We can find a family of unitary operators $\{V(\lambda)\}_{\lambda\in\mathbb{R}}$ on $\mathbb{C}^{N+2}$ such that

$$\varrho(\lambda) = V(\lambda)\begin{pmatrix} \mu_b(\lambda) & 0 & \cdots & \cdots & 0 \\ 0 & \mu_N(\lambda) & 0 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & \cdots & 0 & \mu_1(\lambda) & 0 \\ 0 & \cdots & \cdots & 0 & \mu_a(\lambda) \end{pmatrix} V(\lambda)^*,$$

for a.e. $\lambda \in \mathbb{R}$, where $\mu_\tau(\lambda)$, $\tau = a, 1, \cdots, N, b$, are the non-negative eigenvalues of the matrix $\varrho(\lambda)$. Hence from equation (6.2) we obtain

$$u_\varrho(x,\lambda) = \left\langle \begin{pmatrix} \mu_b(\lambda) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mu_a(\lambda) \end{pmatrix} V(\lambda)^T\Phi(x,\lambda), V(\lambda)^T\Phi(x,\lambda) \right\rangle.$$

Introducing the measurable family of orthogonal bases $\{e^a(\lambda), \cdots, e^b(\lambda)\}_{\lambda\in\mathbb{R}}$, where $e^\tau(\lambda) := V(\lambda)e_\tau$, we find

$$u_\varrho(x,\lambda) = \sum_{\tau=a,\cdots,b} \mu_\tau(\lambda)|\phi(x,\lambda,e^\tau(\lambda))|^2,$$

for $x \in [a,b]$ and $\lambda \in \mathbb{R}$, where we used the fact that

$$V^T(\lambda)\Phi(x,\lambda) = \begin{pmatrix} \phi(x,\lambda,e_b(\lambda)) \\ \vdots \\ \phi(x,\lambda,e_a(\lambda)) \end{pmatrix}. \tag{6.8}$$

7 Current density

We define the current density $j_\varrho(x,\lambda)$ at point x and energy $\lambda \in \mathbb{R}$ of the system described by the dissipative operator H by

$$j_\varrho(x,\lambda) := \sum_{\tau=0}^{N+1} \mu_\tau(\lambda)\operatorname{Im}\left(\frac{1}{m(x)}\phi(x,\lambda,e^\tau(\lambda))'\overline{\phi(x,\lambda,e^\tau(\lambda))}\right). \tag{7.1}$$

See [LL71] for the motivation for this definition. We note that $\phi(x,\lambda,e^\tau(\lambda))'$ exists only for $x \neq x_j$, $j = 1, \cdots, N$. Therefore, the definition (7.1) makes only sense for $x \in \bigcup_{j=0}^{N}(x_j, x_{j+1})$.

Equation (7.1) can be rewritten as

$$j_\varrho(x,\lambda) = \operatorname{Im}\left(\left\langle \varrho(\lambda)^T\frac{1}{m(x)}\Phi(x,\lambda)', \Phi(x,\lambda)\right\rangle\right). \tag{7.2}$$

Finally this can be expressed as

$$j_\varrho(x,\lambda) = \operatorname{tr}(\varrho(\lambda)C(x,\lambda)),$$

where

$$C(x,\lambda) := \operatorname{Im}\begin{pmatrix} \frac{1}{m(x)}\phi(x,\lambda,N+1)'\overline{\phi(x,\lambda,N+1)} & \cdots & \frac{1}{m(x)}\phi(x,\lambda,0)'\overline{\phi(x,\lambda,N+1)} \\ \frac{1}{m(x)}\phi(x,\lambda,N+1)'\overline{\phi(x,\lambda,N)} & \cdots & \frac{1}{m(x)}\phi(x,\lambda,0)'\overline{\phi(x,\lambda,N)} \\ \vdots & & \vdots \\ \frac{1}{m(x)}\phi(x,\lambda,N+1)'\overline{\phi(x,\lambda,0)} & \cdots & \frac{1}{m(x)}\phi(x,\lambda,0)'\overline{\phi(x,\lambda,0)} \end{pmatrix}. \tag{7.3}$$

The current density is strongly related to the characteristic function of the operator H. This is shown in the next theorem.

Theorem 7.1 *Assume that* $m + \frac{1}{m} \in \mathsf{L}^\infty(a,b)$, $V \in \mathsf{L}^2(a,b)$, *with* $\operatorname{Im}(V) = 0$, *and* $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$ *as well as* $x_1, \cdots, x_N \in (a,b)$ *such that* $x_1 < x_2 < \cdots < x_N$. *Let* ϱ *be a steady state. Then the current density* $j_\varrho(x,\lambda)$, $x \in [a,b]$, $x \neq x_j$, $\lambda \in \mathbb{R}$, *is independent of* x *for* $x \in (x_j, x_{j+1})$ *and admits the representation*

$$j_\varrho(x,\lambda) = \operatorname{tr}(\varrho(\lambda)C(x,\lambda)), \tag{7.4}$$

where

$$C(x,\lambda) := \sum_{j=0}^{N} E_j(\lambda)\Theta_H(\lambda)^*\chi_{(x_j,x_{j+1})}(x) \tag{7.5}$$

and

$$E_j(\lambda) := \frac{1}{2\pi}\left(P_-^j\Theta_H(\lambda)P_+^j - P_+^j\Theta_H(\lambda)P_-^j\right) \tag{7.6}$$

with

$$P_-^j := \sum_{z=0}^{j} P_z, \quad P_+^j := \sum_{z=j+1}^{N+1} P_z, \qquad P_z := \langle\cdot, e_z\rangle e_z.$$

Moreover, if $\operatorname{tr}(\varrho(\cdot)) \in \mathsf{L}^1(\mathbb{R})$, *then the total current* $j_\varrho(x)$ *at point* $x \in (x_j, x_{j+1})$,

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

is finite and can be estimated by

$$|j_\varrho(x)| \leq \frac{1}{2\pi}\int_{\mathbb{R}} \operatorname{tr}(\varrho(\lambda))\,d\lambda. \tag{7.7}$$

Proof. We have

$$j_\varrho(x,\lambda) = \operatorname{tr}(\varrho(\lambda)C(x,\lambda)), \tag{7.8}$$

where $C(x,\lambda)$ is given by (7.3). $C(x,\lambda)$ can be rewritten as

$$C(x,\lambda) = \frac{1}{i}\begin{pmatrix} W(\overline{\phi(\cdot,\lambda,N+1)},\phi(\cdot,\lambda,N+1))(x) & \cdots & W(\overline{\phi(\cdot,\lambda,N+1},\phi(\cdot,\lambda,0))(x) \\ W(\overline{\phi(\cdot,\lambda,N)},\phi(\cdot,\lambda,N+1))(x) & \cdots & W(\overline{\phi(\cdot,\lambda,N)},\phi(\cdot,\lambda,0))(x) \\ \vdots & & \vdots \\ W(\overline{\phi(\cdot,\lambda,0)},\phi(\cdot,\lambda,N+1))(x) & \cdots & W(\overline{\phi(\cdot,\lambda,0)},\phi(\cdot,\lambda,0))(x) \end{pmatrix}. \tag{7.9}$$

Clearly $W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)$ is constant for every x in each subinterval (x_j, x_{j+1}), for every $l, m = 0, \cdots, N+1$. Hence, $j_\varrho(x,\lambda)_{|(x_j,x_{j+1})}$ is constant.

Let us compute $C(x,\lambda)_{|(x_j,x_{j+1})}$. Since $\phi(x,\lambda,k)$ has to fulfil the boundary conditions (5.5) and (5.6) (see also figure 1), we get

$$\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} =& W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_j+0)\\
=& W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_j-0)\\
&- i\alpha_j^2\overline{\phi(x_j,\lambda,l)}\phi(x_j,\lambda,m)+\delta_{jm}\frac{\alpha_m}{\sqrt{2\pi}}\overline{\phi(x_m,\lambda,l)}\\
=& W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_{j-1}+0)\\
&- i\alpha_j^2\overline{\phi(x_j,\lambda,l)}\phi(x_j,\lambda,m)+\delta_{jm}\frac{\alpha_m}{\sqrt{2\pi}}\overline{\phi(x_m,\lambda,l)}\\
&\vdots\\
=& \sum_{\tau=0}^{j}\left\{-i\alpha_\tau^2\overline{\phi(x_\tau,\lambda,l)}\phi(x_\tau,\lambda,m)+\delta_{\tau,m}\frac{\alpha_\tau}{\sqrt{2\pi}}\overline{\phi(x_\tau,\lambda,l)}\right\},
\end{aligned}$$

for $l,m=0,\cdots,N+1$ and $l>j$, where $\delta_{\tau,m}=\langle e_\tau,e_m\rangle$. Similar we obtain for all $l,m=0,\cdots,N+1$, $l\le j$,

$$\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} =& W(\overline{\phi(x,\lambda,l)},\phi(x,\lambda,m))(x_{j+1}-0)\\
=& W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_{j+1}+0)\\
&+ i\alpha_{j+1}\overline{\phi(x_{j+1},\lambda,l)}\phi(x_{j+1},\lambda,m)-\delta_{j+1,m}\frac{\alpha_m}{\sqrt{2\pi}}\overline{\phi(x_{j+1},\lambda,l)}\\
=& W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x_{j+2}-0)\\
&+ i\alpha_{j+1}\overline{\phi(x_{j+1},\lambda,l)}\phi(x_{j+1},\lambda,m)-\delta_{j+1,m}\frac{\alpha_m}{\sqrt{2\pi}}\overline{\phi(x_{j+1},\lambda,l)}\\
&\vdots\\
=& \sum_{\tau=j+1}^{N+1}\left\{i\alpha_\tau^2\overline{\phi(x_\tau,\lambda,l)}\phi(x_\tau,\lambda,m)-\delta_{\tau,m}\frac{\alpha_\tau}{\sqrt{2\pi}}\overline{\phi(x_\tau,\lambda,l)}\right\}.
\end{aligned}$$

Note that

$$\frac{1}{\sqrt{2\pi}}\langle\alpha T_*(\lambda)^*e_\xi,e_\tau\rangle=-\alpha_\tau\phi(x_\tau,\lambda,\xi)$$

for all $\tau,\xi=0,\cdots,N+1$. Hence we find

$$\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= \frac{1}{\sqrt{2\pi}}\sum_{\tau=0}^{j}\left\{-i\sqrt{2\pi}\alpha_\tau\phi(x_\tau,\lambda,m)+\delta_{\tau,m}\right\}\alpha_\tau\overline{\phi(x_\tau,\lambda,l)} \qquad (7.10)\\
&= -\frac{1}{2\pi}\sum_{\tau=0}^{j}\{i\langle\alpha T_*(\lambda)^*e_m,e_\tau\rangle+\langle e_m,e_\tau\rangle\}\,\overline{\langle\alpha T_*(\lambda)^*e_l,e_\tau\rangle}
\end{aligned}$$

for $l>j$. Using equation (4.9) we get

$$\begin{aligned}
W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= -\frac{1}{2\pi}\sum_{\tau=0}^{j}\langle\Theta_H(\lambda)^*e_m,e_\tau\rangle\overline{\langle\alpha T_*(\lambda)^*e_l,e_\tau\rangle} \qquad (7.11)\\
&= -\frac{1}{2\pi}\langle P_-^j\Theta_H(\lambda)^*e_m,\alpha T_*(\lambda)^*e_l\rangle
\end{aligned}$$

or

$$W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} = -\frac{i}{2\pi}\langle P_-^j\Theta_H(\lambda)^*e_m,\Theta_H(\lambda)^*P_+^j\ e_l\rangle \qquad (7.12)$$

for $l > j$. If $l \leq j$, then

$$W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} = \frac{1}{\sqrt{2\pi}}\sum_{\tau=j+1}^{N+1}\left\{i\sqrt{2\pi}\alpha_\tau\phi(x_\tau,\lambda,m)-\delta_{\tau,m}\right\}\alpha_\tau\overline{\phi(x_\tau,\lambda,l)} \tag{7.13}$$

$$= \frac{1}{2\pi}\sum_{\tau=j+1}^{N+1}\{i\langle T_*(\lambda)^*e_m,e_\tau\rangle + \langle e_m,e_\tau\rangle\}\overline{\langle \alpha T_*(\lambda)^*e_l,e_\tau\rangle}.$$

Using again (4.9) we obtain

$$\begin{aligned} W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} &= \frac{1}{2\pi}\sum_{\tau=j+1}^{N+1}\langle\Theta_H(\lambda)^*e_m,e_\tau\rangle\overline{\langle\alpha T_*(\lambda)^*e_l,e_\tau\rangle} \\ &= \frac{i}{2\pi}\langle P_+^j\Theta_H(\lambda)^*e_m,\Theta_H(\lambda)^*e_l\rangle \end{aligned} \tag{7.14}$$

which yields

$$W(\overline{\phi(\cdot,\lambda,l)},\phi(\cdot,\lambda,m))(x)_{|(x_j,x_{j+1})} = \frac{i}{2\pi}\langle P_+^j\Theta_H(\lambda)^*e_m,\Theta_H(\lambda)^*P_-^j\; e_l\rangle \tag{7.15}$$

for $l \leq j$. Taking into account (7.9), (7.12) and (7.15) we find

$$\langle C(x,\lambda)e_m,e_l\rangle\rangle_{|(x_j,x_{j+1})} = \frac{1}{2\pi}\left\langle\{P_-^j\Theta_H(\lambda)P_+^j - P_+^j\Theta_H(\lambda)P_-^j\}\Theta_H(\lambda)^*e_m,e_l\right\rangle \tag{7.16}$$

for $m,l = 0,1,\ldots,N+1$. Using notation (7.5) and (7.6) we immediately obtain (7.4).

From the above calculations we get for the total current $j_\varrho(x)$, $x \in (x_j,x_{j+1})$,

$$|j_\varrho(x)| \leq \|\varrho(\lambda)C(x,\lambda)\|_{\mathfrak{B}_1(\mathbb{C}^{N+2})} \leq \frac{1}{2\pi}\|\varrho(\lambda)\|_{\mathfrak{B}_1(\mathbb{C}^{N+2})}\|E_j(\lambda)\|_{\mathfrak{B}(\mathbb{C}^{N+2})}.$$

By (7.6) one gets

$$E_j(\lambda)^*E_j(\lambda) = P_+^j\Theta_H(\lambda)^*P_-^j\Theta_H(\lambda)P_+^j + P_-^j\Theta_H(\lambda)^*P_+^j\Theta_H(\lambda)P_-^j$$

which yields

$$E_j(\lambda)^*E_j(\lambda) \leq I.$$

Hence $\|E_j(\lambda)\|_{\mathfrak{B}(\mathbb{C}^{N+2})} \leq 1$ which verifies (7.7). □

Let us show that piecewise constant matrix-valued function $C(x,\lambda)$ is selfadjoint for each $x \neq x_j$. If $x \in (x_j,x_{j+1})$, then one gets

$$C(x,\lambda)^* = \Theta_H(\lambda)E_j(\lambda)^* = \frac{1}{2\pi}\Theta_H(\lambda)\{P_-^j\Theta_H(\lambda)^*P_+^j - P_+^j\Theta_H(\lambda)^*P_-^j\}.$$

One has

$$\begin{aligned} C(x,\lambda)^* =& \frac{1}{2\pi}\{P_+^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j + P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j \\ &- P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j - P_-^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j\}. \end{aligned}$$

Since $P_+^j + P_-^j = I$ and $\Theta_H(\lambda)\Theta_H(\lambda)^* = I$ we find

$$\begin{aligned} C(x,\lambda)^* =& \frac{1}{2\pi}\{-P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_-^j + P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_-^j \\ &- P_+^j\Theta_H(\lambda)P_-^j\Theta_H(\lambda)^*P_+^j + P_-^j\Theta_H(\lambda)P_+^j\Theta_H(\lambda)^*P_+^j\} \end{aligned}$$

which yields

$$C(x,\lambda)^* = \frac{1}{2\pi}\{P_-^j\Theta_H(\lambda)P_+^j - P_+^j\Theta_H(\lambda)P_-^j\}\Theta_H(\lambda)^* = C(x,\lambda)$$

Since $C(x,\lambda)$ is selfadjoint it is useful, in correspondence to the current density, to make the following definition.

Definition 7.2 The piecewise constant matrix $C(\cdot,\lambda)$ defined by (7.5) is called the current density observable and the piecewise constant function

$$j_\varrho(x,\lambda) = \mathrm{tr}(\varrho(\lambda)C(x,\lambda))$$

is called the current density at point $x \in [a,b]$, $x \neq x_j$, and energy $\lambda \in \mathbb{R}$.

The definition is justified by the fact that the current density is the expectation value of the current density observable at energy $\lambda \in \mathbb{R}$ and point $x \in \mathbb{R}$, i.e. $j_\varrho(x,\lambda) = \mathbb{E}_{\varrho(\lambda)}(C(x,\lambda))$. Using this notion we get

$$j_\varrho(x) = \int_{\mathbb{R}} \mathbb{E}_{\varrho(\lambda)}(C(x,\lambda))\, d\lambda.$$

Let us consider the special case, where the steady state ϱ is a function of K, i.e. $\varrho = f(K)$, for some $f \in \mathsf{L}^\infty(\mathbb{R})$, $f \geq 0$. In this case ϱ belong to the bicommutant of K. As in [KNR01c] we get that in this case the current density is zero. This fact is proven by the following Corollary.

Corollary 7.3 *Suppose that* $m + \frac{1}{m} \in \mathsf{L}^\infty(a,b)$, $V \in \mathsf{L}^2(a,b)$, *such that* $\mathrm{Im}(V) = 0$, $\kappa_a, \kappa_1, \cdots, \kappa_N, \kappa_b \in \mathbb{C}_+$, *as well as* $x_1, \cdots, x_N \in (a,b)$, *with* $x_1 < x_2 < \cdots < x_N$. *Furthermore assume that the steady state* ϱ *is of the form* $\varrho = f(K)$, *where* $f \in \mathsf{L}^\infty(\mathbb{R})$ *is non-negative. Then* $j_\varrho(x,\lambda) = 0$ *for* $x \neq x_\tau$, $\tau = a, x_1, \cdots, x_N, b$, *and a.e.* $\lambda \in \mathbb{R}$.

Proof. Clearly we have $\varrho(\lambda) = f(\lambda) I_{\mathbb{C}^{N+2}}$, $\lambda \in \mathbb{R}$. Thus we get for $x \in (x_j, x_{j+1})$

$$j_\varrho(x,\lambda) = f(\lambda)\mathrm{tr}_{\mathbb{C}^{N+2}}(C(x,\lambda))$$

Using (7.5) and (7.6) we obtain

$$j_\varrho(x,\lambda) = f(\lambda)\mathrm{tr}(E_j(x,\lambda)\Theta_H(\lambda)^*) = f(\lambda)\mathrm{tr}\left(\left(P^j_-\Theta_H(\lambda)P^j_+ - P^j_+\Theta_H(\lambda)P^j_-\right)\Theta_H(\lambda)^*\right).$$

Since

$$\mathrm{tr}\left(P^j_+\Theta_H(\lambda)P^j_-\Theta_H(\lambda)^*\right) = \mathrm{tr}\left(P^j_+\Theta_H(\lambda)P^j_-\Theta_H(\lambda)^*P^j_+\right) = \mathrm{tr}\left(P^j_-\Theta_H(\lambda)^*P^j_+\Theta_H(\lambda)P^j_-\right)$$

and

$$\mathrm{tr}\left(P^j_-\Theta_H(\lambda)P^j_+\Theta_H(\lambda)^*\right) = \mathrm{tr}\left(P^j_-\Theta_H(\lambda)P^j_+\Theta_H(\lambda)^*P^j_-\right)$$

we have

$$\mathrm{tr}\left(\left(P^j_-\Theta_H(\lambda)P^j_+ - P^j_+\Theta_H(\lambda)p^J_-\right)\Theta_H(\lambda)^*\right) = 0$$

which proves $j_\varrho(x,\lambda) = 0$. $\square$

8 Current variations

In Theorem 7.1 we showed that the current density $j_\varrho(x,\lambda)$ is piecewise constant in x. Let us calculate the current difference for some $\tilde{a} \in (x_j, x_{j+1})$ and $\tilde{b} \in (x_{j+1}, x_{j+2})$:

$$\begin{aligned} j_\varrho(\tilde{b},\lambda) - j_\varrho(\tilde{a},\lambda) &= \frac{1}{2\pi}\mathrm{tr}(\varrho(\lambda)\{C_{j+1}(\lambda) - C_j(\lambda)\}) \\ &= \frac{1}{2\pi}\mathrm{tr}(\varrho(\lambda)\{P^{j+1}_-\Theta_H(\lambda)P^{j+1}_- - P^j_-\Theta_H(\lambda)P^j_-\}\Theta^*_H(\lambda)) \\ &= \frac{1}{2\pi}\mathrm{tr}(\varrho(\lambda)\{P_{j+1}\Theta_H(\lambda) - \Theta_H(\lambda)P_{j+1}\}\Theta^*_H(\lambda)) \\ &= \frac{1}{2\pi}\mathrm{tr}(P_{j+1}\{\varrho(\lambda) - \Theta^*(\lambda)\varrho(\lambda)\Theta_H(\lambda)\}P_{j+1}). \qquad (8.1) \end{aligned}$$

More general we get for $\hat{a} \in (x_j, x_{j+1})$ and $\hat{b} \in (x_{j+k+1}, x_{j+k+2})$

$$j_\varrho(\hat{b}, \lambda) - j_\varrho(\hat{a}, \lambda) = \frac{1}{2\pi}\mathrm{tr}(Q\{\varrho(\lambda) - \Theta_H(\lambda)\varrho(\lambda)\Theta_H^*(\lambda)\}Q), \tag{8.2}$$

where $Q = \sum_{\tau=j}^{j+k} P_\tau$.

From equation (8.2) we see that the current difference depends essentially on the density matrix $\varrho(\lambda)$. For example, if $\varrho(\lambda)$ commutes with $\Theta_H(\lambda)$ we get that the difference is zero. Hence, the current is constant. In the case that the difference in (8.2) is positive, the system is "losing" electrons between the points $\tilde{a}$ and $\tilde{b}$. If the difference in (8.2) is negative, the system "gains" electrons. The effect of losing and gaining electrons is closely related to a recombination-generation process.

In the following we are going to construct a density matrix $\varrho(\cdot)$, such that the r.h.s. of (8.2) is expressed in terms of the density $u_\varrho(x_\xi, \lambda)$ and the α_j's.

Let $\mathcal{R}_{\lambda_0}, \mathcal{G}_{\lambda_0} \subseteq \{1, \cdots, N\} := \mathcal{T}$ such that $\mathcal{R}_{\lambda_0} \cap \mathcal{G}_{\lambda_0} = \emptyset$, $\mathcal{R}_{\lambda_0} \cup \mathcal{G}_{\lambda_0} = \mathcal{T}$, and $u(\lambda_0) \in \mathbb{C}^{N+2}$ with

$$\langle u(\lambda_0), e_\tau\rangle = 0, \quad \forall \tau \in \mathcal{R}_{\lambda_0}, \text{ and } \langle u(\lambda_0), \Theta_H(\lambda_0)e_\tau\rangle = 0, \quad \forall \tau \in \mathcal{G}_{\lambda_0}, \tag{8.3}$$

where $\lambda_0 \in \mathbb{R}$ is fixed. We define the operator $\varrho(\lambda_0)$ by

$$\varrho(\lambda_0)^T := \overline{u(\lambda_0)}u(\lambda_0)^T.$$

The function $f(x, \lambda_0)$ given by

$$\begin{pmatrix} 0 \\ \vdots \\ 0 \\ f(x,\lambda_0) \end{pmatrix} = u(\lambda_0)^T\Phi(x, \lambda),$$

satisfies the following boundary conditions:

$$\Delta(f(\cdot, \lambda_0))(x_\tau) = -\kappa_\tau f(x_\tau, \lambda_0), \quad \forall \tau \in \mathcal{R}_{\lambda_0}, \tag{8.4}$$

$$\Delta(f(\cdot, \lambda_0))(x_\xi) = -\overline{\kappa_\xi} f(x_\xi, \lambda_0), \quad \forall \xi \in \mathcal{G}_{\lambda_0}. \tag{8.5}$$

Let $\omega = [\tilde{a}, \tilde{b}] \subseteq \Omega$ be a given interval and $\mathcal{T}_\omega := \{j \in \mathcal{T} \,|\, x_j \in \omega\}$. The current difference is then given by

$$\begin{aligned} j_\varrho(\tilde{b}, \lambda_0) - j_\varrho(\tilde{a}, \lambda_0) =& \mathrm{Im}\left(\left\langle u(\lambda_0)^T \frac{1}{m(\tilde{b})}\Phi(\tilde{b}, \lambda_0)', u(\lambda_0)^T\Phi(\tilde{b}, \lambda_0)\right\rangle\right) \\ &- \mathrm{Im}\left(\left\langle u(\lambda_0)^T \frac{1}{m(\tilde{a})}\Phi(\tilde{a}, \lambda_0)', u(\lambda_0)^T\Phi(\tilde{a}, \lambda_0)\right\rangle\right) \\ =& \frac{1}{i}\sum_{\tau\in\mathcal{T}_\omega}\left\{W(\overline{f(\cdot, \lambda_0)}, f(\cdot, \lambda_0))(x_\tau + 0) - W(\overline{f(\cdot, \lambda_0)}, f(\cdot, \lambda_0))(x_\tau - 0)\right\}. \end{aligned}$$

Using the boundary conditions (8.4) and (8.5) we obtain

$$\begin{aligned} j_\varrho(\tilde{b}, \lambda_0) - j_\varrho(\tilde{a}, \lambda_0) &= \sum_{\tau\in\mathcal{T}_\omega\cap\mathcal{G}_{\lambda_0}} \alpha_\tau^2|f(x_\tau, \lambda_0)|^2 - \sum_{\xi\in\mathcal{T}_\omega\cap\mathcal{R}_{\lambda_0}} \alpha_\xi^2|f(x_\xi, \lambda_0)|^2 \\ &= \sum_{\tau\in\mathcal{T}_\omega\cap\mathcal{G}_{\lambda_0}} \alpha_\tau^2\,\langle V(\lambda_0)\Phi(x_\tau, \lambda_0), V(\lambda_0)\Phi(x_\tau, \lambda_0)\rangle \\ &\quad - \sum_{\xi\in\mathcal{T}_\omega\cap\mathcal{R}_{\lambda_0}} \alpha_\xi^2\,\langle V(\lambda_0)\Phi(x_\xi, \lambda_0), V(\lambda_0)\Phi(x_\xi, \lambda_0)\rangle \\ &= \sum_{\tau\in\mathcal{T}_\omega\cap\mathcal{G}_{\lambda_0}} \alpha_\tau^2 u_\varrho(x_\tau, \lambda_0) - \sum_{\xi\in\mathcal{T}_\omega\cap\mathcal{R}_{\lambda_0}} \alpha_\xi^2 u_\varrho(x_\xi, \lambda_0). \end{aligned}$$

Clearly a vector $u(\lambda_0)$ with the properties (8.3) always exists. In the following we will construct a vector $u(\lambda_0)$ for almost every $\lambda_0 \in \mathbb{R}$, such that $u(\lambda_0)$ is determined up to two given parameters. Let $u_a(\lambda_0), u_b(\lambda_0) \in \mathbb{C}$ be arbitrary. We are now going to construct the vector $u(\lambda_0) = (u^a(\lambda_0), \cdots, u^b(\lambda_0))^T$.

We set $P_{\mathcal{G}_{\lambda_0}} := \sum_{j \in \mathcal{G}_{\lambda_0}} P_j$ and $m_{\mathcal{G}_{\lambda_0}} := \#\mathcal{G}_{\lambda_0}$, i.e. the number of elements in $\mathcal{G}_{\lambda_0}$.

The first condition in (8.3) implies that $u^j(\lambda_0) = 0$ for $j \in \mathcal{R}_{\lambda_0}$. Furthermore we set $u^a(\lambda_0) = u_a(\lambda_0)$ and $u^b(\lambda_0) = u_b(\lambda_0)$. The second condition in (8.3) can be rewritten to

$$P_{\mathcal{G}_{\lambda_0}} \Theta_H(\lambda_0)^* P_{\mathcal{G}_{\lambda_0}} u = -\left(u_b(\lambda_0) P_{\mathcal{G}_{\lambda_0}} \Theta_H(\lambda_0)^* e_b + u_a(\lambda_0) P_{\mathcal{G}_{\lambda_0}} \Theta_H(\lambda_0)^* e_a\right). \tag{8.6}$$

Since $P_{\mathcal{G}_{\lambda_0}} \Theta_H(\lambda_0)^* P_{\mathcal{G}_{\lambda_0}}$ can be seen as a $m_{\mathcal{G}_{\lambda_0}} \times m_{\mathcal{G}_{\lambda_0}}$-matrix, the equation (8.6) has a solution for a.e. λ_0 if

$$\det_{m_{\mathcal{G}_{\lambda_0}}}(P_{\mathcal{G}_{\lambda_0}} \Theta_H(\lambda_0)^* P_{\mathcal{G}_{\lambda_0}}) \neq 0,$$

where $\det_{m_{\mathcal{G}_{\lambda_0}}}(\cdot)$ denotes the determinant in the vector space $\mathbb{C}^{m_{\mathcal{G}_{\lambda_0}}}$.

Since $\langle \Theta_H(\cdot) e_j, e_k \rangle$ is a bounded analytic function on $\overline{\mathbb{C}_-}$ (cf. [FN70]), we get that $\det_{m_{\mathcal{G}_{\lambda_0}}}(\cdot)$ is also a bounded analytic function on $\overline{\mathbb{C}_-}$. Hence $\det_{m_{\mathcal{G}_{\lambda_0}}}(\Theta_H(\lambda)) \neq 0$ for a.e. λ_0.

The remaining components of u, i.e. u^j, $j \in \mathcal{G}_{\lambda_0}$, are then determined as the solution of the linear equation (8.6).

Thus we proved that we can construct a density matrix $\varrho(\lambda_0)$ for a.e. λ_0, such that we obtain a loss and gain effect at predefined points x_j. Furthermore we showed that one has two degrees of freedom in the choice of $\varrho(\lambda_0)$, namely $u^b(\lambda_0)$ and $u^a(\lambda_0)$.

By repeating the above procedure for every $\lambda \in \mathbb{R}$ we can construct a density matrix $\varrho(\lambda)$, for every $\lambda \in \mathbb{R}$. It can easily be seen that the condition (6.1) is satisfied if $u^a(\lambda)$ and $u^b(\lambda)$ decay sufficiently fast, e.g. $u^a(\lambda), u^b(\lambda)$ have compact support.

We will give some examples: Assume that $u^b(\lambda_0), u^a(\lambda_0) \in \mathbb{C}$ are given and let $\mathcal{R}_{\lambda_0} = \{1, \cdots, N\}$, $\mathcal{G}_{\lambda_0} = \emptyset$. Clearly the vector

$$u_R(\lambda_0) := (u^b(\lambda_0), 0, \cdots, 0, u^a(\lambda_0))^T$$

satisfies equation (8.3). Introducing the density matrix by

$$\varrho_R(\lambda_0)^T := \overline{u_R(\lambda_0)} u_R(\lambda_0)^T,$$

we get

$$j_{\varrho_R}(\tilde{b}, \lambda_0) - j_{\varrho_R}(\tilde{a}, \lambda_0) = -\sum_{\tau=1}^{N} \alpha_\tau^2 u_{\varrho_R}(x_\tau, \lambda_0),$$

i.e. the density matrix $\varrho_R(\lambda_0)$ is purely recombinative.

To obtain a density matrix which is purely generative we introduce the vector

$$u_G(\lambda_0) := \Theta_H(\lambda_0) u_R(\lambda_0),$$

which satisfies equation (8.3) with $\mathcal{R}_{\lambda_0} = \emptyset$ and $\mathcal{G}_{\lambda_0} = \{1, \cdots, N\}$. As above we define the density matrix by $\varrho_G(\lambda_0)^T := \overline{u_G(\lambda_0)} u_G(\lambda_0)^T$ and get

$$j_{\varrho_G}(\tilde{b}, \lambda_0) - j_{\varrho_G}(\tilde{a}, \lambda_0) = \sum_{\tau=1}^{N} \alpha_\tau^2 u_{\varrho_G}(x_\tau, \lambda_0).$$

Thus $\varrho_G(\lambda_0)$ is purely generative. We note that

$$\varrho_G(\lambda_0) = \Theta_H(\lambda_0) \varrho_R(\lambda_0) \Theta_H(\lambda_0)^*. \tag{8.7}$$

9 Remarks

The definition of carrier and current density was formulated in terms of the complete orthonormal system of eigenfunctions $\{\vec{\phi}(\cdot,\lambda,a),\cdots,\vec{\phi}(\cdot,\lambda,b)\}_{\lambda\in\mathbb{R}}$. Since the eigenfunctions behave on $\mathbb{R}_-$ like free wave, they are called the incoming eigenfunctions. By equation (5.10) we can define another system of orthogonal eigenfunctions by

$$\vec{\phi}_{\mathrm{out}}(\cdot,\lambda,j) := \frac{1}{\sqrt{2\pi}}\vec{\phi}^{\Theta(\lambda)e_j}(\cdot,\lambda), \quad j = 0,\cdots,N+1,$$

which are called the outgoing eigenfunctions. By equation (6.8) the following relation holds

$$\Theta_H(\lambda)\Phi_{\mathrm{in}}(x,\lambda) = \begin{pmatrix} \phi_{\mathrm{out}}(x,\lambda,b) \\ \vdots \\ \phi_{\mathrm{out}}(x,\lambda,a) \end{pmatrix} := \Phi_{\mathrm{out}}(x,\lambda), \tag{9.1}$$

where we have set $\Phi_{\mathrm{in}}(x,\lambda) = \Phi(x,\lambda)$.

Using the outgoing eigenfunction we define the "outgoing" carrier and current density by

$$\begin{aligned} u_\varrho^{\mathrm{out}}(x,\lambda) &:= \left\langle \varrho(\lambda)^T\Phi_{\mathrm{out}}(x,\lambda), \Phi_{\mathrm{out}}(x,\lambda)\right\rangle, \\ j_\varrho^{\mathrm{out}}(x,\lambda) &:= \mathrm{Im}\left\langle \varrho(\lambda)^T\frac{1}{m(x)}\Phi_{\mathrm{out}}(x,\lambda)', \Phi_{\mathrm{out}}(x,\lambda)\right\rangle \end{aligned}$$

Using (9.1) we get

$$u_\varrho^{\mathrm{out}}(x,\lambda) = u^{\mathrm{in}}_{\Theta_H\varrho\Theta_H^*}(x,\lambda), \quad j_\varrho^{\mathrm{out}}(x,\lambda) = j^{\mathrm{in}}_{\Theta_H\varrho\Theta_H^*}(x,\lambda),$$

where $u_\varrho^{\mathrm{in}}(x,\lambda)$, $j_\varrho^{\mathrm{in}}(x,\lambda)$ denotes the carrier, respectively current, density defined in the previous sections.

The incoming and the outgoing carrier and current densities coincide, if $\varrho(\lambda)$ commutes with the characteristic function $\Theta_H(\lambda)$. As already mentioned above in this case neither loss nor gain effects will occur.

In the previous section we gave an example for a purely recombinative density matrix $\varrho_R(\lambda)$ and an example for a strict generative matrix $\varrho_G(\lambda)$. Using the relations (9.1) and (8.7) we get

$$j^{\mathrm{in}}_{\varrho_G}(x,\lambda) = j^{\mathrm{out}}_{\varrho_R}(x,\lambda).$$

i.e. the generative matrix ϱ_G in the incoming representation becomes a recombinative matrix in the outgoing representation.

Introducing the notions $P_j^{\mathrm{in}} = \langle\cdot,e_j\rangle e_j$ and $P_j^{\mathrm{out}} = \langle\cdot,E_j\rangle E_j$, where $E_j = \Theta_H^*(\lambda)e_j$, we can rewrite (8.1) as follows

$$j_\varrho(\tilde{b},\lambda) - j_\varrho(\tilde{a},\lambda) = \frac{1}{2\pi}\mathrm{tr}(\varrho(\lambda)\{P_j^{\mathrm{in}} - P_j^{\mathrm{out}}\}).$$

Let us consider two different dissipative Schrödinger operator H_n and H_p for the two different species of particles (electron and holes), with m_n, m_p, V_n, V_p, $\kappa_{j,n}$, $\kappa_{j,p}$, $j = 1,\cdots,N$, and let x_j, $j = 1,\cdots,N$, be numbers within the interval (a,b) such that $a < x_1 < \cdots < x_N < b$. We denote by $u_{\varrho_k}(x,\lambda)$, respectively $j_{\varrho_k}(x,\lambda)$, the carrier density, respectively current density, corresponding to the density matrix ϱ_k and the operator H_k, $k = n,p$.

Assume that the sets $\mathcal{G}_\lambda = \mathcal{G}$ and $\mathcal{R}_\lambda = \mathcal{R}$ are given. Let $\varrho_n(\lambda)$ and $\varrho_p(\lambda)$ density matrices satisfying equation (6.1) such that

$$j_{\varrho_n}(\tilde{b},\lambda) - j_{\varrho_n}(\tilde{a},\lambda) = \sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega} \alpha^2_{\tau,n} u_{\varrho_n}(x_\tau,\lambda) - \sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega} \alpha^2_{\xi,n} u_{\varrho_n}(x_\xi,\lambda), \qquad \text{for a.e.} \quad \lambda\in\mathbb{R} \tag{9.2}$$

$$j_{\varrho_p}(\tilde{b},\lambda) - j_{\varrho_p}(\tilde{a},\lambda) = -\left(\sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega} \alpha^2_{\tau,p} u_{\varrho_p}(x_\tau,\lambda) - \sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega} \alpha^2_{\xi,p} u_{\varrho_p}(x_\xi,\lambda)\right), \qquad \text{for a.e.} \quad \lambda\in\mathbb{R}. \tag{9.3}$$

By the consideration of section 8, such density matrices exists. Integrating (9.2) and (9.3) with respect to λ yields

$$j_{\varrho_n}(\tilde{b}) - j_{\varrho_n}(\tilde{a}) = \sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega} \alpha^2_{\tau,n} u_{\varrho_n}(x_\tau) - \sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega} \alpha^2_{\xi,n} u_{\varrho_n}(x_\xi,), \tag{9.4}$$

$$j_{\varrho_p}(\tilde{b}) - j_{\varrho_p}(\tilde{a}) = -\left(\sum_{\tau\in\mathcal{R}\cap\mathcal{T}_\omega} \alpha^2_{\tau,p} u_{\varrho_p}(x_\tau) - \sum_{\xi\in\mathcal{G}\cap\mathcal{T}_\omega} \alpha^2_{\xi,p} u_{\varrho_p}(x_\xi)\right). \tag{9.5}$$

Integrating the stationary continuity equation (cf. (1.3)) over ω gives

$$j_{\varrho_n}(\tilde{b}) - j_{\varrho_n}(\tilde{a}) = -\left(j_{\varrho_p}(\tilde{b}) - j_{\varrho_p}(\tilde{a})\right) \tag{9.6}$$

Matching equation (9.6) with (9.4) and (9.5) leads to a condition on the $\alpha^2_{j,n}$'s and $\alpha^2_{j,p}$'s, i.e.

$$\alpha^2_{j,n} = u_{\varrho_p}(x_j,\lambda), \quad \text{and} \quad \alpha^2_{j,p} = u_{\varrho_n}(x_j,\lambda), \quad j = 1,\cdots,N. \tag{9.7}$$

The equations (9.4),(9.5) can now be viewed as a stationary continuity equation with recombination-generation term given by

$$\int_\omega R(u_{\varrho_n}(x), u_{\varrho_p}(x))\,dx = \sum_{j\in\mathcal{T}_\omega\cap\mathcal{R}} u_{\varrho_n}(x_j)u_{\varrho_p}(x_j) - \sum_{j\in\mathcal{T}_\omega\cap\mathcal{G}} u_{\varrho_n}(x_j)u_{\varrho_p}(x_j).$$

To solve the nonlinear equation given by (9.7) we introduce the operators $\mathcal{N}_k : \mathbb{R}^N_+ \to \mathbb{R}^N_+$, given by

$$\mathcal{N}_k(\alpha^2_{1,k},\cdots,\alpha^2_{N,k}) = (u_{\varrho_k}(x_1),\cdots,u_{\varrho_k}(x_N)),$$

where $k = n, p$.

A solution of (9.7) is thus given by a fix point of the operator $\mathcal{E}$ defined by

$$\mathcal{E}(\alpha^2_{1,n},\cdots,\alpha^2_{N,n}) := \mathcal{N}_p(\mathcal{N}_n(\alpha^2_{1,n},\cdots,\alpha^2_{N,n})).$$

As in [KNR01c, BKNR02a] one can set up a dissipative Schrödinger-Poisson system using the definition of carrier densities introduced in this article. In addition to the Schrödinger-Poisson system considered in [BKNR02a] the current is not constant. This system will be discussed in a forthcoming paper.

In section 8 we constructed explicitly a density matrix $\varrho(\cdot)$ such that loss and gain effects occur at predefined points. Furthermore we showed that one has two free parameters in the choice of $\varrho(\cdot)$, i.e. $u_b(\lambda)$ and $u_a(\lambda)$. These two parameters give the possibility to couple (for example) a drift diffusion model to the open quantum system. We intend to investigate this coupled system in a forthcoming paper.

For simplicity we considered imaginary potentials of the form $-\frac{\alpha^2}{2}\delta(\cdot - x_j)$. A further step in order to include recombination and generation into the model is to allow complex potentials, i.e. $\mathrm{Im}(V) = -\frac{\alpha^2}{2}$, where $\alpha = \alpha(x) \in \mathsf{L}^p$ for some $p > 1$. This would give the possibility to model recombination-generation rates on the whole interval Ω.

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