1   Introduction

Nowadays semiconductor device technology permits to fabricate devices whose size is of a few nanometers only. In these devices the particle can no longer move freely in all space directions and thus the description of a three–dimensional electron gas is not adequate anymore. Consequently, van Roosbroeck's drift–diffusion model [72] does not properly describe the physical phenomena and a finer level of modeling has to be used.

The Schrödinger operator is one of the fundamental tools for the understanding and prediction of nanoscaled semiconductor devices. The one–particle Schrödinger operators in effective–mass approximation for electrons (superscript "$-$") and holes (superscript "$+$") are given by

$$H^{\pm}\psi = -\frac{\hbar^2}{2}\nabla \cdot \left[(\mathbf{m}^{\pm})^{-1}\nabla\psi\right] + V^{\pm}\psi, \tag{1.1a}$$

where $\hbar$ is the reduced Planck constant, $\mathbf{m}^{\pm} = \mathbf{m}^{\pm}(x)$ are the mass tensors, and $V^{\pm}$ are the potential energies of electron and holes, respectively. The potentials $V^{\pm}$ are real–valued and split up into the electrostatic potential φ and the heterostructure potentials $V_h^{\pm}$, i.e.

$$V^{\pm} = V_h^{\pm} \pm \mathrm{q}\varphi. \tag{$*$}$$

The natural space to consider the operators (1.1a) is the Hilbert space $\mathcal{H} = \mathsf{L}^2(\Omega;\mathbb{C})$, i.e. the space of complex–valued square integrable functions, where $\Omega \subset \mathbb{R}^d$, $d \leq 3$, denotes the bounded spatial domain occupied by the semiconductor device. Depending on the physical situation, boundary conditions for the Schrödinger operator (1.1a) are imposed on the boundary of Ω. Moreover, the electrostatic potential φ has to be determined by a Poisson equation

$$-\nabla \cdot \left(\boldsymbol{\epsilon}\,\nabla\varphi\right) = \mathrm{q}\left(N_D + u^+ - u^-\right) \qquad \text{on } \Omega, \tag{1.1b}$$

where $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}(x)$ denotes the dielectric permittivity tensor and N_D the doping profile of the semiconductor device. The Poisson equation (1.1b) is usually supplemented by mixed boundary conditions allowing Ohmic—metal—contacts on some part of the boundary while other parts are insulated, see [34, 69]. The densities $u^{\pm}$ on the right hand side of the Poisson equation (1.1b) depend on the spectral properties of the Schrödinger operators (1.1a) and given statistics. Since the Schrödinger operators depend on the electrostatic potential, see ($*$), the densities $u^{\pm}$ depend on φ, too. Consequently, the Schrödinger operators (1.1a) and the Poisson equation (1.1b) are coupled in a non–linear way. Systems of this type are called *Schrödinger–Poisson systems*.

The mathematical analysis of Schrödinger–Poisson systems in the past years, focused mainly on the case of thermodynamic equilibrium [58, 59, 44, 45, 46, 22]. In thermodynamic equilibrium the boundary conditions for the Schrödinger operator (1.1a) are of mixed Dirichlet Neumann type, which make the Schrödinger operators (1.1a) selfadjoint. Let us denote these selfadjoint Schrödinger operators by $H_{\mathrm{th}}^{\pm}$. The selfadjoint operators $H_{\mathrm{th}}^{\pm}$ are regarded as Hamiltonians of the corresponding quantum system

for electrons and holes. The statistical operators $\varrho_{\text{th}}^{\pm}$ in thermodynamic equilibrium are given as a function of the corresponding Hamiltonian, i.e.

$$\varrho_{\text{th}}^{\pm} = \mathscr{F}^{\pm}\left(H_{\text{th}}^{\pm} - E_F^{\pm}\right), \tag{1.2a}$$

where $E_F^{\pm}$ are the constant Fermi level characterizing the thermodynamic equilibrium of the semiconductor under consideration. The functions $\mathscr{F}^{\pm}$ are (reduced) equilibrium distribution functions, like Boltzmann or Fermi–Dirac distribution functions. The statistical operators $\varrho_{\text{th}}^{\pm}$ are non–negative trace class operators. Moreover, $\varrho_{\text{th}}^{\pm}$ commute with $H_{\text{th}}^{\pm}$ and are therefore solutions of the corresponding *stationary von Neumann equation*

$$[H_{\text{th}}^{\pm}, \varrho_{\text{th}}^{\pm}] = 0, \tag{1.2b}$$

where $[\cdot, \cdot]$ denotes the usual commutator bracket. Non–negative trace class operators $\varrho_{\text{th}}^{\pm}$ that satisfy the stationary von Neumann equations (1.2b) are called *steady states* of $H_{\text{th}}^{\pm}$. The integral kernels of $\varrho_{\text{th}}^{\pm}$, denoted by $\boldsymbol{\varrho}_{\text{th}}^{\pm}(x, y)$, i.e.

$$\left(\varrho_{\text{th}}^{\pm} f\right)(x) = \int_{\Omega} \boldsymbol{\varrho}_{\text{th}}^{\pm}(x, y) f(y) \, \mathrm{d}y, \qquad x \in \Omega, \text{ for all } f \in \mathcal{H} = \mathsf{L}^2(\Omega; \mathbb{C}), \tag{1.2c}$$

are called *density matrices* for electrons and holes, respectively. The particle densities $u_{\text{th}}^{\pm}$ are then given by

$$u_{\text{th}}^{\pm}(x) = \boldsymbol{\varrho}_{\text{th}}^{\pm}(x, x), \qquad x \in \Omega. \tag{1.2d}$$

The Schrödinger–Poisson system constituting of a Poisson equation (1.1b), where the densities on the right hand side are given by the expressions (1.2d), i.e. comprising selfadjoint Schrödinger operators (1.1a) and steady states of the form (1.2a), is called the *Schrödinger–Poisson system in thermodynamic equilibrium.*

In 1990 Nier [59] showed that the mapping

$$\mathcal{V} \ni \varphi \mapsto -\nabla \cdot \left(\boldsymbol{\epsilon} \, \nabla \varphi\right) + \mathrm{q} \, u_{\text{th}}^{-}[\varphi] - \mathrm{q} \, u_{\text{th}}^{+}[\varphi] \in \mathcal{V}^*,$$

is a strictly monotone potential operator, see also [41]. Here $\mathcal{V}$ is a Sobolev space, depending on the boundary conditions imposed on (1.1b), $\mathcal{V}^*$ the corresponding dual space and $u_{\text{th}}^{\pm}[\varphi]$ indicates the dependence of the densities $u_{\text{th}}^{\pm}$ from (1.2d) on the electrostatic potential φ. The monotonicity implies that the Schrödinger–Poisson system in thermodynamic equilibrium admits a unique solution φ, see also [22, 58, 59, 44, 45, 46, 41].

In order to describe a semiconductor device away from thermodynamic equilibrium one has to take into account the interaction of the device with its environment e.g. batteries at the contacts, etc. The exchange of particles of the device with the contacts results in a current flowing through the boundary of the device domain. Therefore, one has to consider *open quantum systems*. Mixed Dirichlet Neumann boundary conditions for the Schrödinger equation (1.1a) cannot describe a current flow through the boundary of the device and are thus not adequate to describe an open system. In fact quantum systems comprising selfadjoint Schrödinger operators are always closed, see [68, 29]. Thus, to describe open quantum systems one has to consider boundary conditions for the Schrödinger operators (1.1a), which make the operators non–selfadjoint on $\mathcal{H} = \mathsf{L}^2(\Omega; \mathbb{C})$. Let us denote these non–selfadjoint operators by $H_{\text{open}}^{\pm}$.

The Schrödinger operators $H_{\mathrm{open}}^{\pm}$ cannot be regarded as Hamiltonians of the quantum systems in the usual sense, see [68], and thus it is not clear how to define the macroscopic quantities such as particle and current density for an open quantum systems. To overcome this difficulty one assumes that the open quantum systems described by the non–selfadjoint Schrödinger operators $H_{\mathrm{open}}^{\pm}$ on the Hilbert space $\mathcal{H} = \mathsf{L}^2(\Omega; \mathbb{C})$ can be embedded into a larger closed quantum system described by selfadjoint operators $K^{\pm}$ on some Hilbert space $\mathcal{K}$. Mathematically this embedding is expressed by the following conditions:

(i) the Hilbert space $\mathcal{K}$ contains the Hilbert space $\mathcal{H}$ as a subspace, and

(ii) the following relation holds:

$$(H_{\mathrm{open}}^{\pm} - z)^{-1} = P_{\mathcal{K}}^{\mathcal{H}}(K^{\pm} - z)^{-1} \restriction \mathcal{H}, \tag{1.3a}$$

where $H_{\mathrm{open}}^{\pm}$ denotes the non–selfadjoint Schrödinger operators associated to the open quantum system, $K^{\pm}$ are selfadjoint operators on the Hilbert space $\mathcal{K}$, $P_{\mathcal{H}}^{\mathcal{K}}$ denotes the orthogonal projection from $\mathcal{K}$ onto $\mathcal{H}$, and $\restriction \mathcal{H}$ indicates the restriction to the Hilbert space $\mathcal{H}$.

If the conditions (i) and (ii) hold, the the non–selfadjoint Schrödinger operators $H_{\mathrm{open}}^{\pm}$ on $\mathcal{H}$ are called *pseudo Hamiltonians* of the open quantum system and the selfadjoint operators $K^{\pm}$ on $\mathcal{K}$ are called *quasi Hamiltonians*, see e.g. [29].

The macroscopic quantities for the open quantum system are then constructed as follows: Let $\varrho^{\pm}$ be steady states of $K^{\pm}$, that is non–negative operators which commute with $K^{\pm}$, i.e.

$$[K^{\pm}, \varrho^{\pm}] = 0. \tag{1.3b}$$

The steady states $\varrho_{\mathrm{open}}^{\pm}$ for the open quantum system are then defined by

$$\varrho_{\mathrm{open}}^{\pm} = P_{\mathcal{H}}^{\mathcal{K}} \varrho^{\pm} \restriction \mathcal{H}, \tag{1.3c}$$

which are assumed to be non–negative trace class operators on $\mathcal{H} = \mathsf{L}^2(\Omega; \mathbb{C})$.

Away from equilibrium one cannot assume that the operators $\varrho^{\pm}$ are functions of the quasi Hamiltonians $K^{\pm}$, see (1.2a). In fact one needs a non–equilibrium theory, see e.g. [39], in order to determine the steady states $\varrho^{\pm}$. The condition (1.3b) does not determine the steady states uniquely.

The *density matrices* $\boldsymbol{\varrho}_{\mathrm{open}}^{\pm}(x, y)$ for the open quantum system are then given as the integral kernels of $\varrho_{\mathrm{open}}^{\pm}$, i.e.

$$\left(\varrho_{\mathrm{open}}^{\pm} f\right)(x) = \int_{\Omega} \boldsymbol{\varrho}_{\mathrm{open}}^{\pm}(x, y) f(y) \, \mathrm{d}y, \qquad x \in \Omega, \text{ for all } f \in \mathcal{H} = \mathsf{L}^2(\Omega; \mathbb{C}). \tag{1.3d}$$

The densities of electrons u_{open}^{-} and holes u_{open}^{+} for the open systems are obtained by

$$u_{\mathrm{open}}^{\pm}(x) = \boldsymbol{\varrho}_{\mathrm{open}}^{\pm}(x, x), \qquad x \in \Omega. \tag{1.3e}$$

The electrostatic potential φ has to be determined selfconsistently by the Poisson equation (1.1b), where the densities $u^{\pm}$ on the right hand side are given by the expressions $u_{\mathrm{open}}^{\pm}$ from equation (1.3e).

The system consisting of a Poisson equation where the densities on the right hand side are determined by means of Schrödinger operators $H_{\mathrm{open}}^{\pm}$ which are pseudo Hamiltonians of open quantum systems are called *open Schrödinger–Poisson systems.* The present thesis is devoted to this type of Schrödinger–Poisson systems in a one–dimensional setting.

The thesis is organized as follows: First we introduce some notation. In Section 2 we introduce a general class of dissipative Schrödinger operators, which play a center role in the analysis of open Schrödinger–Poisson systems. In Section 3 we consider the dissipative Schrödinger–Poisson system, where the pseudo Hamiltonians of the open quantum systems are given by maximal dissipative Schrödinger operators as introduced in Section 2. In Section 4 we present the analysis of the quantum transmitting Schrödinger–Poisson system. Here the the pseudo Hamiltonians of the open quantum systems are given by families of maximal dissipative operators, the so called quantum transmitting boundary families. In Section 5 we present a model which consists of an open quantum model coupled to a classical drift–diffusion model. Moreover, we show that the model is capable to describe the transport in a resonant tunneling structure.

Each section ends with a subsection which summarizes the results of the section and gives an outlook on possible forthcoming research.

1.1   Notation

In the following we introduce some general notation, which we need in the sequel. Note that a list of symbols can be found on page 143.

Numbers and sets. $\mathbb{N}$ denotes the natural numbers $1, 2, 3, \ldots$. $\mathbb{R}$, $\mathbb{C}$ are the real and complex numbers, respectively. The real and imaginary part of a number $z \in \mathbb{C}$ is written as $\mathfrak{Re}(z)$ and $\mathfrak{Im}(z)$, respectively. We define $\mathbb{C}_+ \overset{\mathrm{def}}{=} \{z \in \mathbb{C} \,|\, \mathfrak{Im}(z) > 0\}$ and similarly $\mathbb{C}_- \overset{\mathrm{def}}{=} \{z \in \mathbb{C} \,|\, \mathfrak{Im}(z) < 0\}$. The imaginary unit is denoted by i and the complex conjugated for some $z \in \mathbb{C}$ is indicated by $\overline{z}$. The characteristic function of a set ω is denoted by χ_ω, i.e. $\chi_\omega(x) = 1$ if $x \in \omega$ and $\chi_\omega(x) = 0$ else. The closure of a set ω is written as $\mathrm{clo}(\omega)$. If $\Sigma = (a, b) \subset \mathbb{R}$ is any interval, then we denote by $\partial \Sigma \overset{\mathrm{def}}{=} \{a, b\}$ the boundary and by $|\Sigma| \overset{\mathrm{def}}{=} b - a$ the length of this interval.

Banach and Hilbert spaces.   The norm of a Banach space $\mathscr{X}$ is denoted by $\|\cdot\|_{\mathscr{X}}$ and the adjoint space is indicated by $\mathscr{X}^*$. For vectors $f, f_n \in \mathscr{X}$, $n \in \mathbb{N}$, we denote by $f = \lim_{n \to \infty} f_n$ of $f_n \to f$, $n \to \infty$, the convergence in the $\|\cdot\|_{\mathscr{X}}$–norm (strong convergence). Let $\mathcal{I}$ be any index set and $f_i \in \mathscr{X}$, $i \in \mathcal{I}$, given vectors. The closed linear span of the family $\{f_i\}_{i \in \mathcal{I}}$ is denoted by $\mathrm{clospan}_{i \in \mathcal{I}} f_i$. If $\mathscr{H}$ is a Hilbert space, then $\langle \cdot, \cdot \rangle_{\mathscr{H}}$ denotes the scalar product, where the first argument is the linear one. In this paper a Hilbert space is always assumed to be separable. By $\{e_j \,|\, j = 1 \ldots, k\}$, we denote the canonical basis of the Hilbert space $\mathbb{C}^k$ and by P_j, $j = 1, \ldots, k$ the corresponding projection on the subspace spanned by e_j, i.e. $P_j = \langle \cdot, e_j \rangle_{\mathbb{C}^k} e_j$.

Operators on Banach spaces. Let $\mathscr{X}$, $\mathscr{Y}$ be Banach spaces. $\mathrm{dom}(A)$ denotes the domain of an operator $A : \mathscr{X} \longrightarrow \mathscr{Y}$ and its range is indicated by $\mathrm{ran}(A)$. The restriction of an operator A to a subset $\mathscr{S}$ of $\mathrm{dom}(A)$ is written as $A \upharpoonright \mathscr{S}$. Moreover, if A is a densely defined linear operator, we denote by A^* its adjoint operator. The notations $\mathrm{spec}(A)$ and $\mathrm{res}(A)$ refer to the spectrum and resolvent sets of A, respectively. The Banach space of all bounded linear operators A is denoted by $\mathfrak{B}(\mathscr{X};\mathscr{Y})$, with norm $\|\cdot\|_{\mathfrak{B}(\mathscr{X};\mathscr{Y})}$. In the special case where $\mathscr{X} = \mathscr{Y}$ we simply write $\mathfrak{B}(\mathscr{X})$ and $\|\cdot\|_{\mathfrak{B}(\mathscr{X})}$ instead of $\mathfrak{B}(\mathscr{X};\mathscr{X})$ and $\|\cdot\|_{\mathfrak{B}(\mathscr{X};\mathscr{X})}$. Moreover, in this case $\mathbb{I}_{\mathscr{X}}$ is the identity operator. For linear operators $A, A_n : \mathscr{X} \longrightarrow \mathscr{Y}$, $n \in \mathbb{N}$, we denote by $A = \lim_{n\to\infty} A_n$, $A = \operatorname*{s\text{-}lim}_{n\to\infty} A_n$, and $A = \operatorname*{w\text{-}lim}_{n\to\infty} A_n$, the (operator) norm, strong, and weak convergence of A_n to A, respectively. Occasionally we also write $A_n \to A$, $A_n \xrightarrow{\mathrm{s}} A$, and $A_n \xrightarrow{\mathrm{w}} A$, $n \to \infty$, for the norm, strong and weak convergence, respectively.

Operators on Hilbert spaces. Let $\mathscr{H}$ and $\mathscr{K}$ be Hilbert spaces. The trace of a linear operator $A : \mathscr{H} \longrightarrow \mathscr{K}$, if it exists, is referred to as $\mathrm{tr}(A)$. If, moreover, A is densely defined and closed, then $|A|$ denotes the absolute value of A. By $\mathfrak{B}_1(\mathscr{H};\mathscr{K})$ we denote the set of all trace class operators from $\mathscr{H}$ to $\mathscr{K}$ and $\|\cdot\|_{\mathfrak{B}_1(\mathscr{H};\mathscr{K})}$ is the corresponding trace norm. The set of all Hilbert–Schmidt operator is written as $\mathfrak{B}_2(\mathscr{H};\mathscr{K})$ and $\|\cdot\|_{\mathfrak{B}_2(\mathscr{H};\mathscr{K})}$ refers to the corresponding Hilbert–Schmidt norm. If $\mathscr{H} = \mathscr{K}$ we abbreviate $\mathfrak{B}_1(\mathscr{H}) = \mathfrak{B}_1(\mathscr{H};\mathscr{H})$ and $\mathfrak{B}_2(\mathscr{H}) = \mathfrak{B}_2(\mathscr{H};\mathscr{H})$. Let $A : \mathscr{H} \longrightarrow \mathscr{H}$ be a selfadjoint operator, then $\mathrm{spec}_{\mathrm{ac}}(A)$ and $\mathrm{spec}_{\mathrm{p}}(A)$ denote the absolutely continuous and pure point spectrum of A. The point and absolutely continuous subspaces of A are denoted by $\mathscr{H}_{\mathrm{p}}(A)$ and $\mathscr{H}_{\mathrm{ac}}(A)$, respectively. The projections on the corresponding subspaces are indicated by $P_{\mathrm{p}}(A)$, $P_{\mathrm{ac}}(A)$, respectively.

L^p spaces. Let $\Sigma \subseteq \mathbb{R}$ and ν be a measure. Then, we denote as usual by $\mathsf{L}^p(\Sigma; \mathscr{X}; \nu)$, $1 \leq p < \infty$, the space of ν–measurable, p–(Bochner) integrable functions with values in the Banach space $\mathscr{X}$. $\mathsf{L}^\infty(\Sigma; \mathscr{X}; \nu)$ is the corresponding set of essentially bounded functions. If ν is the Lebesgue measure, we simply write $\mathsf{L}^p(\Sigma; \mathscr{X})$, $1 < p \leq \infty$.

Space of continuous functions and Sobolev spaces. Let $\Sigma \subseteq \mathbb{R}$ be an interval and $\mathscr{X}$ be a Banach space. The space of continuous functions $f : \Sigma \longrightarrow \mathscr{X}$ is denoted as usual by $\mathsf{C}(\Sigma; \mathscr{X})$ and by $\mathsf{C}_0^\infty(\Sigma; \mathscr{X})$ the space smooth functions with compact support. We denote by $\mathsf{W}^{r,p}(\Sigma; \mathscr{X})$ the usual Sobolev space of r times weak differentiable and p–integrable (with respect to the Lebesgue measure) functions.

Let $\Gamma \subseteq \partial\Sigma$ be a subset of the boundary. If $\mathscr{X} = \mathbb{R}$, we denote by $\mathsf{W}_\Gamma^{1,2}(\Sigma; \mathbb{R}) \overset{\mathrm{def}}{=} \{f \in \mathsf{W}^{1,2}(\Sigma; \mathbb{R}) \,|\, f(\Gamma) \subset \{0\}\}$. If $\Gamma = \partial\Sigma$, then we abbreviate $\mathsf{W}_0^{1,2}(\Sigma; \mathbb{R})$ for $\mathsf{W}_\Gamma^{1,2}(\Sigma; \mathbb{R})$. The dual space of $\mathsf{W}^{1,2}(\Sigma; \mathbb{R})$ is denoted as usual by $\mathsf{W}^{-1,2}(\Sigma; \mathbb{R})$. The dual paring between $\mathsf{W}^{1,2}(\Sigma; \mathbb{R})$ and $\mathsf{W}^{-1,2}(\Sigma; \mathbb{R})$ is denoted by $\langle \cdot, \cdot \rangle_{\mathsf{W}^{1,2}, \mathsf{W}^{-1,2}}$. Analogous we write $\mathsf{W}_\Gamma^{-1,2}(\Sigma; \mathbb{R})$, $\mathsf{W}_0^{-1,2}(\Sigma; \mathbb{R})$ for dual of $\mathsf{W}_\Gamma^{1,2}(\Sigma; \mathbb{R})$ and $\mathsf{W}_0^{1,2}(\Sigma; \mathbb{R})$, respectively. $\langle \cdot, \cdot \rangle_{\mathsf{W}_\Gamma^{1,2}, \mathsf{W}_\Gamma^{-1,2}}$ and $\langle \cdot, \cdot \rangle_{\mathsf{W}_0^{1,2}, \mathsf{W}_0^{-1,2}}$ denote the corresponding dual parings.

Embedding operators. Let $\Sigma \subset \mathbb{R}$ be a bounded interval and $\Gamma \subseteq \partial\Sigma$ a subset of the boundary. The embedding operator form $\mathsf{L}^1(\Sigma; \mathbb{R})$ into $\mathsf{W}_\Gamma^{-1,2}(\Sigma; \mathbb{R})$ is denoted by

$I_{1,\Sigma,\Gamma}$. Moreover, we write $\iota_{1,\Sigma,\Gamma}$ for its norm. The embedding operator from $\mathsf{W}^{1,2}(\Sigma;\mathbb{R})$ into $\mathsf{L}^\infty(\Sigma;\mathbb{R})$ is denoted by $I_{\infty,\Sigma}$ and its norm is abbreviated by $\iota_{\infty,\Sigma}$. If $\Gamma = \partial\Sigma$, then we abbreviate $I_{1,\Sigma}$ and $\iota_{1,\Sigma}$ for $I_{1,\Sigma,\partial\Sigma}$ and $\iota_{1,\Sigma,\partial\Sigma}$.

Multiplication operators. Let $\mathfrak{V} \in \mathsf{L}^\infty(\Sigma; \mathfrak{B}(\mathscr{X}); \nu)$, where $\Sigma \subseteq \mathbb{R}$, $\mathscr{X}$ is some Banach space, and ν some measure. The linear and bounded multiplication operator induced by $\mathfrak{V}$ on the Hilbert space $\mathsf{L}^2(\Sigma; \mathscr{X}; \nu)$ is denoted by $M(\mathfrak{V})$, i.e. $M(\mathfrak{V}) \in \mathfrak{B}(\mathsf{L}^2(\Sigma; \mathscr{X}; \nu))$ is given by $(M(\mathfrak{V})f)(x) \stackrel{\text{def}}{=} \mathfrak{V}(x)f(x)$, $x \in \Sigma$, $f \in \mathrm{dom}(M(\mathfrak{V})) = \mathsf{L}^2(\Sigma; \mathscr{X}; \nu)$. Note that $\|M(\mathfrak{V})\|_{\mathfrak{B}(\mathsf{L}^2(\Sigma;\mathscr{X};\nu))} = \|\mathfrak{V}\|_{\mathsf{L}^\infty(\Sigma;\mathfrak{B}(\mathscr{X});\nu)}$. To simplify the notation, we use the following convention: If it is clear from the context, we do not distinguish between the operator $M(\mathfrak{V})$ and the function $\mathfrak{V}$ and simply write $\mathfrak{V}$ also for the operator $M(\mathfrak{V})$.

Physical constants. The reduced Planck constant is denoted as usual by $\hbar$. The (positive) elementary charge is denoted by q. Boltzmann's constant is denoted by k_B and the constant temperature by T. The electron rest mass is denoted by m_0 and the permittivity in vacuum is indicated by ϵ_0. The values of the constants are listed in Table 1 and are taken from standard text books, e.g. [54, 68, 50].

Quantity	Symbol	Value
Boltzmann constant	k_B	$1.38 \cdot 10^{-23}\text{VAs/K}$
Electron rest mass	m_0	$0.91 \cdot 10^{-20}\text{kg}$
Elementary charge	q	$1.6 \cdot 10^{-19}\text{As}$
Permittivity in vacuum	ϵ_0	$8.85 \cdot 10^{-14}\text{AsV}^{-1}\text{cm}^{-1}$
Reduced Planck constant	$\hbar$	$1.05 \cdot 10^{-34}\text{VAs}^2$

Table 1: *Physical constants.*

2   A class of dissipative Schrödinger operators

In this section we introduce a general class of dissipative Schrödinger operators, which play a central role in our further considerations. The section is organized as follows: In Subsection 2.1 we state the assumptions, define the class of maximal dissipative Schrödinger operators, and give some properties of these operators. In Subsection 2.2 we explicitly determine the characteristic function and the selfadjoint dilation corresponding to the dissipative Schrödinger operators introduced before. Additionally, we determine the Fourier transform of the dilation. Subsection 2.3 is devoted to some mathematical scattering theory for the selfadjoint dilation. In Subsection 2.4 we consider an example of a dissipative Schrödinger operator. We close the section with some notes.

Before defining the Schrödinger operator, which we are going to consider here, we recall some basic definitions and theorems of dissipative operators, see [70, 29, 25].

Definition 2.1. *Let A be a closed operator with domain $\mathrm{dom}(A)$ dense in a Hilbert space $\mathscr{H}$. A is called* dissipative, *if*

$$\mathfrak{Im}\left(\langle Af, f\rangle_{\mathscr{H}}\right) \leq 0 \quad \textit{for every } f \in \mathrm{dom}(A).$$

A is called maximal dissipative, *if it has no proper dissipative extension.*

A is said to be completely non–selfadjoint, *if there exists no non–zero reducing subspace $\mathscr{H}'$ of $\mathscr{H}$ such that $A \upharpoonright (\mathrm{dom}(A) \cap \mathscr{H}')$ is a selfadjoint operator.*

The spectrum of a dissipative operator A is contained in the lower half plane, i.e. $\mathrm{spec}(A) \subseteq \mathrm{clo}(\mathbb{C}_-)$. Moreover, the estimate $\|(A - z)^{-1}\|_{\mathfrak{B}(\mathscr{H})} \leq 1/\mathfrak{Im}(z)$, for all $z \in \mathbb{C}_+$, holds.

An important theorem in the theory of maximal dissipative operators is the Dilation Theorem, which assigns a selfadjoint operator to a maximal dissipative operator.

Theorem 2.2 (Dilation Theorem). *Let A be a maximal dissipative operator on a Hilbert space $\mathscr{H}$. There exists a larger Hilbert space $\mathscr{K}$ containing $\mathscr{H}$ as a subspace, i.e. $\mathscr{H} \subseteq \mathscr{K}$, and a selfadjoint operator B on $\mathscr{K}$ such that the following relation holds*

$$P_{\mathscr{H}}^{\mathscr{K}}(B - z)^{-1} \upharpoonright \mathscr{H} = (A - z)^{-1}, \quad \textit{for all } z \in \mathbb{C}_+,$$

where $P_{\mathscr{H}}^{\mathscr{K}}$ denotes the projection from $\mathscr{K}$ on $\mathscr{H}$. Moreover, the minimality condition

$$\operatorname*{clospan}_{z \in \mathbb{C} \backslash \mathbb{R}} (B - z)^{-1} \mathscr{H} = \mathscr{K}$$

holds. B and $\mathscr{K}$ are unique up to isomorphisms. B is called the minimal selfadjoint dilation *corresponding to A.*

Note that if A is selfadjoint on $\mathscr{H}$, then the minimal selfadjoint dilation corresponding to A is A itself.

Another important object when dealing with dissipative operators is the characteristic function. Let us assume that A is a maximal dissipative operator on a Hilbert space $\mathscr{H}$. We introduce the *Cayley transform C_A* corresponding to A by

$$C_A \overset{\mathrm{def}}{=} (A + \mathrm{i})(A - \mathrm{i})^{-1}. \tag{2.1}$$

Since A is assumed to be maximal dissipative, we have that C_A is a contraction, i.e. $\|C_A f\|_{\mathscr{H}} \leq \|f\|_{\mathscr{H}}$ and 1 is not an eigenvalue of C_A, see [70, Theorem IV.4.1.]. Therfore, $A = \mathrm{i}(C_A + 1)(C_A - 1)^{-1}$. Note that C_A is unitary, if and only if A is selfadjoint. In what follows we will assume that A is dissipative and completely non–selfadjoint. The *defect operators* D_A, D_A' and the *defect spaces* $\mathscr{D}_A$, $\mathscr{D}_A'$ are defined by

$$D_A \overset{\text{def}}{=} (1 - C_A^* C_A)^{1/2}, \quad D_A' \overset{\text{def}}{=} (1 - C_A C_A^*)^{1/2},$$
$$\mathscr{D}_A \overset{\text{def}}{=} \mathrm{clo}\big(\mathrm{ran}(D_A)\big), \qquad \mathscr{D}_A' \overset{\text{def}}{=} \mathrm{clo}\big(\mathrm{ran}(D_A')\big). \tag{2.2}$$

We define the function

$$\Xi_{C_A}(\xi) \overset{\text{def}}{=} [-C_A + \xi D_A'(1 - \xi C_A^*)^{-1} D_A] \upharpoonright \mathscr{D}_A, \tag{2.3}$$

for all complex ξ for which $1 - \xi C_A^*$ is boundedly invertible, see [70, Chapter VI]. The values of $\Xi_{C_A}(\xi)$ are bounded operators from $\mathscr{D}_A$ into $\mathscr{D}_A'$. $\|\Xi_{C_A}(\xi)f\|_{\mathscr{H}} < \|f\|_{\mathscr{H}}$ for all $f \in \mathscr{D}_A$ and $\xi \in \mathbb{D} = \{z \in \mathbb{C} \,|\, |z| < 1\}$, i.e. Ξ_{C_A} is a purely contractive analytic function on $\mathbb{D}$. Moreover, $\Xi_{C_A}(\xi)^{-1} = \Xi_{C_A}(\xi)^*$ for all ξ with $|\xi| = 1$ and $\xi \in \mathrm{res}(C_A)$. We are now able to define the characteristic function of a maximal dissipative operator.

Definition 2.3. *Let A be a maximal dissipative and completely non–selfadjoint operator on a Hilbert space $\mathscr{H}$. The function $\Xi_A : \mathrm{clo}(\mathbb{C}_-) \longrightarrow \mathfrak{B}(\mathscr{D}_A', \mathscr{D}_A)$ defined by*

$$\Xi_A(z) \overset{\text{def}}{=} \Xi_{C_A}\left(\frac{z + \mathrm{i}}{z - \mathrm{i}}\right), \qquad z \in \mathrm{clo}(\mathbb{C}_-) \tag{2.4}$$

is called the characteristic function *of A.*

By the definition of the characteristic function of A and the properties of the function $\Xi_{C_A}(\xi)$ introduced above, we have that $\Xi_A(z)$ is a contraction for $z \in \mathrm{clo}(\mathbb{C}_-)$ and a unitary operator for real z in the resolvent set of H, i.e.

$$\Xi_A(z)\Xi_A(z)^* = \mathbb{I}_{\mathscr{D}_A'} \quad \text{and} \quad \Xi_A(z)^*\Xi_A(z) = \mathbb{I}_{\mathscr{D}_A} \quad \text{for } z \in \mathbb{R} \cap \mathrm{res}(H). \tag{2.5}$$

The characteristic function of a completely non–selfadjoint operator plays a similar role as the spectral family for a selfadjoint operator, i.e. it contains essentially all information of the operator, see [70, Theorem VI.3.1.].

Additionally we need the definition of coinciding operator valued functions, see [70, p. 192].

Definition 2.4. *We say that two functions $\Theta_1 : \mathrm{clo}(\mathbb{C}_-) \longrightarrow \mathfrak{B}(\mathscr{D}_1', \mathscr{D}_1)$, and $\Theta_2 : \mathrm{clo}(\mathbb{C}_-) \longrightarrow \mathfrak{B}(\mathscr{D}_2', \mathscr{D}_2)$ coincide, if there exist unitary operators $U : \mathscr{D}_1 \longrightarrow \mathscr{D}_2$ and $U' : \mathscr{D}_1' \longrightarrow \mathscr{D}_2'$ such that $\Theta_2(z) = U'\Theta_1(z)U^{-1}$ for all z.*

2.1 Dissipative Schrödinger operator

Before defining the dissipative Schrödinger operator, let us make some general assumptions to which we will refer to in the sequel.