Preface

Downscaling of semiconductor devices, which is now reaching the nanometer scale, makes it mandatory for us to understand the quantum phenomena involved in charge transport. Indeed, for nanoscale devices, the quantum nature of electrons cannot be neglected. In fact, it underlies the operation of an increasing number of devices. Unlike classical transport, the intuition of the physicist and the engineer is becoming insufficient for predicting the nature of device operation in the quantum context—the need for sufficiently accurate and numerically tractable models represents an outstanding challenge in which applied mathematics can play an important role.

The CIME Session "Quantum Transport: Modelling, Analysis and Asymptotics", which took place in Cetraro (Cosenza), Italy, from September 11 to September 16, 2006, was intended both to present an overview of up-to-date mathematical problems in this field and to provide the audience with techniques borrowed from other fields of application.

It was attended by about 50 scientists and researchers, coming from different countries. The list of participants is included at the end of this book.

The school was structured into four courses:

- **Grégoire Allaire** (École Polytechnique, Palaiseau, France) *Periodic Homogeneization and Effective Mass Theorems for the Schrödinger Equation.*
- **Anton Arnold** (Technische Universität, Vienna) *Mathematical Properties of Quantum Evolution Equations.*
- **Pierre Degond** (Université Paul Sabatier and CNRS, Toulouse, France) *Quantum Hydrodynamic and Diffusion Models Derived from the Entropy Principle.*
- **Thomas Yizhao Hou** (Caltech, Los Angeles, USA) *Multiscale Computations for Flow and Transport in Heterogeneous Media.*

This book contains the texts of the four series of lectures presented at the Summer School. Here follows a brief description of the subjects of these courses.

The first course, titled *Periodic Homogeneization and Effective Mass Theorems for the Schrödinger Equation*, was given by Professor Grégoire Allaire, a renowned specialist in homegeneization theory, and introduced the audience to the theory of homogeneization, a powerful tool for mathematically analyzing the multiscale aspects which are encountered in mathematical physics. First, the heuristic method of two-scale asymptotic expansions is discussed, then an entire section is devoted to the rigorous aspects and the main theoretical results that are at the root of the two-scale convergence. Such a method can be applied to the homogeneization of partial differential equations with periodically oscillating coefficients, like the model problem of diffusion in a periodic medium. These tools are then used to derive rigorously the so-called effective mass approximation which justifies the averaging of the crystal lattice effect on the transport of electrons in solids.

The course *Mathematical Properties of Quantum Evolution Equations*, given by Professor Anton Arnold, was aimed at introducing the basic mathematical properties of quantum evolution equations, such as the Schrödinger equation, the von Neumann equation and the Wigner formalism, and also dealt with the modelling of electron injection from reservoirs into semiconductor nano-devices, and the mathematical and numerical analysis of open boundary conditions for such equations. For the Schrödinger–Poisson analysis Strichartz inequalities are presented. In the density matrix formalism, both closed and open quantum systems can be treated. Their evolution is discussed in the space of trace class operators and energy subspaces, employing Lieb–Thirring inequalities. For the analysis of the Wigner–Poisson–Fokker–Planck system, quantum kinetic dispersion estimates are derived for Wigner–Poisson systems, inspired by the Vlasov–Poisson case. In this course, standard dispersion inequalities for the Schrödinger equation and novel stability properties of discrete artificial boundary conditions obtained by Professor Arnold are shown.

The course *Quantum Hydrodynamic and Diffusion Models Derived from the Entropy Principle*, given by Professor Pierre Degond, presents a novel methodology for the derivation of quantum macroscopic equations from kinetic-type models which is based on a deep understanding of the analogy between classical and quantum dynamics. The entropy minimization strategy of Levermore is considered in the quantum context, and is shown to produce diffusion or hydrodynamic-type equations in which the quantum features appear in particular in the nonlocal character of the relationship between the macroscopic variables such as the particle density and the entropic ones such as the chemical potential. The ad hoc corrections of classical fluid equations, which are commonly used in engineering simulations, are clarified and corrected using this approach. They appear as expansions of the fully quantum models in powers of the Planck constant. A whole field of difficult mathematical problems is open for researchers.

The last course was dedicated to numerical issues. In this course, titled *Multiscale Computations for Flow and Transport in Heterogeneous Media* and given by Professor Thomas Hou, a leader in this field, multiscale finite element methods are presented, analysed and illustrated in various physical situations. The author presents an exhaustive review of the more important recent advances in developing multiscale finite element methods for flow and transport in strongly heterogeneous porous media. The applications targeted by this course are in domains other than quantum transport, but the methodology will be of great interest to researchers involved in quantum transport modelling. Indeed, one of the main features of the quantum transport problem is the existence of different scales: macroscopic scales which are related to electrostatic forces and microscopic scales connected to oscillations of single wave functions and at which interference effects take place. Standard numerical methods need mesh sizes at microscopic scales, thus leading to unnecessarily high numerical cost. The goal of the course is to present methods that capture the small-scale effect on the large scales, but do not require resolving all the small-scale features. The course presented novel numerical multiscale methods which allow the use of coarse meshes while succeeding in resolving the microscopic scales.

The school succeeded in introducing the basic mathematical techniques to analyze quantum transport, to present new models dealing with collisions in the quantum context and to enlarge the knowledge in the domain to multiscale techniques borrowed from other fields of applied mathematics. The choice of the courses and the speakers was suggested by the demand of exhaustively presenting the state of art of quantum transport modelling, proposing both the kinetic and the hydrodynamic models, as well as the analytical and numerical aspects of the more significant problems.

During the course, the Thursday afternoon was dedicated to a poster session, where some of the young participants had the opportunity to show their more recent research and to discuss it with all the participants. The contributors to the poster session were D. Finco, E. Kalligiannaki, O. Maj, C. Manzini, O. Morandi, J.P. Milišic, C. Negulescu, G. Panati, T. Ryabukha, M. Schulte, and V.O. Shtyk.

The directors of this course thank the members of the CIME Scientific Committee for their invitation to organize it, and the Director, Professor Pietro Zecca, and the Secretary, Professor Elvira Mascolo, for their continuous help in the organization.

A special thanks has to be addressed to the lecturers for their good presentations, which stimulated scientific discussions. A thanks has to be addressed also to the attending people, constantly animated with genuine interest. The presence of some participants specialist in quantum transport topics favoured interactions among the students, and we are grateful for the attention paid by a precise and careful audience.

We also like to thank MIP Toulouse for its financial support of the French participants.

Finally, we thank the Director and all the staff of Hotel San Michele in Cetraro for their warm hospitality, which greatly contributed to the friendly atmosphere among all the participants.

Toulouse and Firenze, March 2007 *Naoufel Ben Abdallah*
Giovanni Frosali

Mathematical Properties of Quantum Evolution Equations

Anton Arnold

Abstract This chapter focuses on the mathematical analysis of nonlinear quantum transport equations that appear in the modeling of nano-scale semiconductor devices. We start with a brief introduction on quantum devices like the resonant tunneling diode and quantum waveguides. For the mathematical analysis of quantum evolution equations we shall mostly focus on whole space problems to avoid the technicalities due to boundary conditions. We shall discuss three different quantum descriptions: Schrödinger wave functions, density matrices, and Wigner functions. For the Schrödinger–Poisson analysis (in H^1 and L^2) we present Strichartz inequalities. As for density matrices, we discuss both closed and open quantum systems (in Lindblad form). Their evolution is analyzed in the space of trace class operators and energy subspaces, employing Lieb–Thirring-type inequalities. For the analysis of the Wigner–Poisson–Fokker–Planck system we shall first derive (quantum) kinetic dispersion estimates (for Vlasov–Poisson and Wigner–Poisson). The large-time behavior of the linear Wigner–Fokker–Planck equation is based on the (parabolic) entropy method. Finally, we discuss boundary value problems in the Wigner framework.

List of Abbreviations and Symbols

$\Re$	Real part of a complex number
$\Im$	Imaginary part of a complex number
$\bar{z}$	Complex conjugate of $z \in \mathbb{C}$
$\mathcal{F}$, $\mathcal{F}_x$, $\mathcal{F}_{x\to\xi}$	Fourier transform (w.r.t. the x variable; from the x to the ξ variable)

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$\mathcal{F}^{-1}, \mathcal{F}_{\xi\to x}^{-1}$	Inverse Fourier transform (from the ξ to the x variable)
$\hat{\varphi}$	Fourier transform of the function φ, i.e. $\hat{\varphi}(\xi) = (2\pi)^{-N/2}\int_{\mathbb{R}^N}\varphi(x)\mathrm{e}^{-\mathrm{i}x\cdot\xi}\mathrm{d}x$
ℓ^p	Sequence spaces, $1 \le p \le \infty$
$L^p(\Omega)$	Lebesgue spaces on the open set Ω, $1 \le p \le \infty$
$L^p_{loc}(\Omega)$	Spaces of locally p-integrable functions, $1 \le p \le \infty$
$L^p(\Omega, \mathrm{d}\mu)$	Lebesgue spaces on the open set Ω w.r.t. the measure $\mathrm{d}\mu$, $1 \le p \le \infty$
$H^k(\mathbb{R}^N)$	Sobolev spaces on $\mathbb{R}^N$ with differentiability index $k \in \mathbb{Z}$ (and integrability $p = 2$)
$W^{k,p}(\mathbb{R}; X)$	Sobolev spaces of functions on $\mathbb{R}$ with values in the Banach space X (differentiability index $k \in \mathbb{N}_0$, integrability $1 \le p \le \infty$)
$L^{q,p}$	$:= L^q(\mathbb{R}; L^p(\mathbb{R}^N))$, $1 \le q, p \le \infty$
$L^{q,p}_T$	$:= L^q((-T,T); L^p(\mathbb{R}^N))$, with some fixed $T > 0$
$L^1_x(L^q_v)$	$:= L^1(\mathbb{R}^N_x; L^q(\mathbb{R}^N_v))$, $1 \le q \le \infty$
$C(\mathbb{R}; X)$	Space of continuous functions on $\mathbb{R}$ with values in the Banach space X
$C^1(\mathbb{R}; X)$	Space of continuously differentiable functions on $\mathbb{R}$ with values in the normed space X
$C_0(\Omega)$	Continuous functions on Ω with compact support
$C_0^\infty(\Omega)$	Infinitely differentiable functions on Ω with compact support
$C_B^\infty(\Omega)$	Infinitely differentiable, bounded functions on Ω
$\mathcal{S}(\mathbb{R}^N)$	Schwartz space of rapidly decreasing functions on $\mathbb{R}^N$
$\mathcal{S}'(\mathbb{R}^N)$	Tempered distributions on $\mathbb{R}^N$
$\mathcal{B}(X, Y)$	Space of bounded operators from the Banach space X to the Banach space Y
$\mathcal{J}_1(\mathcal{H})$	Space of trace class operators on the Hilbert space $\mathcal{H}$
$\tilde{\mathcal{J}}_1(\mathcal{H})$	(Sub)space of self-adjoint operators trace class operators on the Hilbert space $\mathcal{H}$
$\mathcal{J}_2(\mathcal{H})$	Space of Hilbert–Schmidt operators on the Hilbert space $\mathcal{H}$
Tr	Operator trace
$\Vert\!\vert\!\Vert \cdot \Vert\!\vert\!\Vert_1$	Trace class norm on $\mathcal{J}_1(\mathcal{H})$
$\Vert\!\vert\!\Vert \cdot \Vert\!\vert\!\Vert_2$	Hilbert–Schmidt norm on $\mathcal{J}_2(\mathcal{H})$
x, y	Position variables, x, $y \in \mathbb{R}^N$
v	Velocity variable, $v \in \mathbb{R}^N$
p	Momentum, $p \in \mathbb{R}^N$
t	Time, $t \in \mathbb{R}$
$\hbar$	(Reduced) Planck constant
ε	Permittivity
e	(Positive) elementary charge
m	Particle mass (electron mass, e.g.)
$V(x,t)$	(Electrostatic) potential, $V \in \mathbb{R}$
$\psi(x,t)$	(Schrödinger) wave function, $\psi \in \mathbb{C}$

$w(x,v,t)$	Wigner function, $w \in \mathbb{R}$
$n(x,t)$	(Spatial) position density, $n \geq 0$
$e_{kin}(x,t)$	Kinetic energy density, $e_{kin} \geq 0$
$j(x,t)$	Current density, $j \in \mathbb{R}$
$D(x)$	Doping profile, density of donor ions, $D \geq 0$
$\varrho(x,y,t)$	Density matrix function, $\varrho \in \mathbb{C}$
$\hat{\varrho}$	Density matrix operator, $\hat{\varrho} \in \mathcal{J}_1$
$\mathcal{D}(A)$	Domain of the operator A
$\bar{A}$	Closure of the operator A
A^*	Adjoint of the operator A
$\hookrightarrow$	Continuous embedding of normed spaces
$f *_x g$	(Partial) Convolution of the functions f and g w.r.t. the x variable

1 Quantum Transport Models for Semiconductor Nano-Devices

The modern computer and telecommunication industry relies heavily on the use of semiconductor devices like transistors. A very important fact of the success of these devices is their rapidly shrinking size. Presently, their characteristic size (channel lengths in transistors, e.g.) has been decreased to some deca-nanometers only. On such small length scales, quantum properties of electrons and atoms cannot be neglected any longer and there are two different consequences: On the one hand classical simulation models of "conventional" devices must then be modified as to include quantum corrections. This concerns devices like the *metal oxide semiconductor field-effect transistor* (MOSFET), which is the dominant building block of today's integrated circuits. On the other hand, more and more *intrinsic quantum devices* (like resonant tunneling diodes, resonant tunneling field-effect transistors, single-electron transistors, quantum dots, quantum waveguides) are devised and manufactured. Their main operational features depend on actively exploiting quantum mechanical effects like tunneling, spatial confinements, and quantized energy levels. Such quantum devices have already applications as high frequency oscillators, in laser diodes, and as memory devices. Moreover, quantum dots are very promising candidates for use in solid-state quantum computation. Compared to off-the-shelf MOSFETs, however, they are still used in rather experimental settings with niche applications. But their great technological and commercial potential drives a tremendous research interest in such nano-devices.

The development of novel semiconductor devices is usually supported by computer simulations to optimize the desired operating features. Now, in order to perform the numerical simulations for the electron flow through

a device, mathematical equations (mostly partial differential or integro-differential equations) are needed. They should be both physically accurate and numerically solvable with low computational cost. Semiconductor engineers use various quantum mechanical frameworks in their quantum transport models: Schrödinger wave functions, Wigner functions, density matrices, and Green's functions. Schrödinger models are used to describe the purely ballistic transport of electrons and holes, and they are employed for simulations of quantum waveguides and nano-scale semiconductor heterostructures, e.g. As soon as scattering mechanisms (between electrons and phonons, or with crystal impurities, e.g.) become important, it is convenient to adopt the Wigner formalism or the equivalent density matrix formalism. For practical applications Wigner functions have also the advantage to allow for a rather simple, intuitive formulation of boundary conditions at device contacts or interfaces. As a drawback, the Wigner equation is posed in a high dimensional phase space which makes its numerical solution extremely costly. As a compromise, fluid-type models can provide a reasonable approximation. Although less accurate, they are often used.

In these lecture notes we shall give a survey on the analytical problems and properties associated with Schrödinger, Wigner, and density matrix models that are used in quantum transport applications. For a basic introduction (both physical and mathematical) to quantum mechanics we refer the reader to [Boh89], [LL85], [Deg], Sect. I.6 of [DL88], and [Tha05]. An introduction to quantum transport for semiconductor devices can be found in [Fre94], [Rin03], Sects. 1.4–1.6 of [MRS90], and [KN06].

Before starting the mathematical analysis of quantum evolution equations, we first present the transport models used for two prototype devices – quantum waveguides and resonant tunneling diodes.

1.1 Quantum Waveguide with Adjustable Cavity

In this subsection we discuss the mathematical models used in the simulations of *quantum waveguides*. These are novel electronic switches of nanoscale dimensions. They are made of several different layers of semiconductor materials such that the electron flow is confined to small channels or waveguides. Due to their sandwiched structure the relevant geometry for the electron current is essentially two dimensional. Figure 1 shows the example of a T-shaped *quantum interference transistor*. The actual structure can be realized as an etched layer of GaAs (gallium arsenide) between two layers of doped AlGaAs (aluminum gallium arsenide). Applying an external potential at the gate (i.e. above the shaded portion of the stub), the "allowed region" for the electrons, and hence the geometry (in particular the stub length) can be modified. This allows to control the current flow through such an electronic device. It makes it a switch, which resembles a transistor – but on a nano-scale. With respect

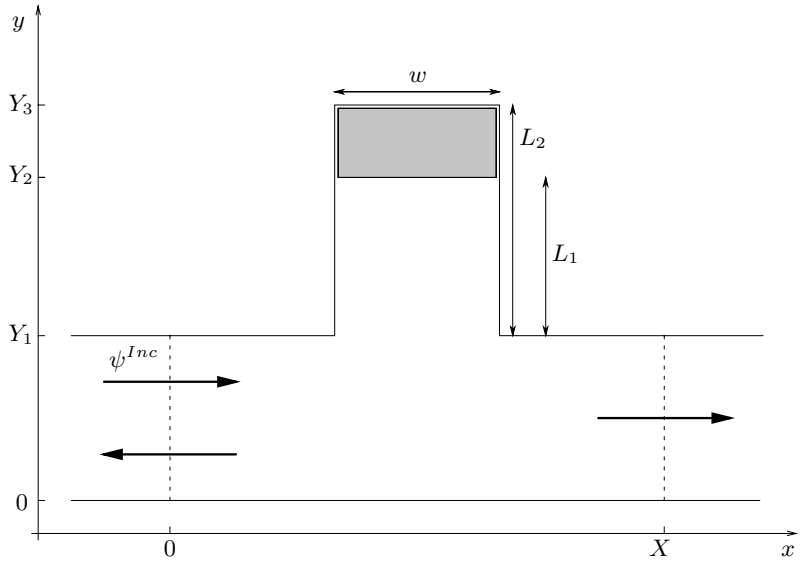

Fig. 1 T-shaped geometry $\Omega \subset \mathbb{R}^2$ of a quantum interference transistor with source and drain contacts to the left and right of the channel. Applying a gate voltage above the stub allows to modify the stub length from L_1 to L_2 and hence to switch the transistor between the on- and off-states. In numerical simulations, the domain Ω is artificially cut off at $x = 0$ and $x = X$ by adding transparent boundary conditions

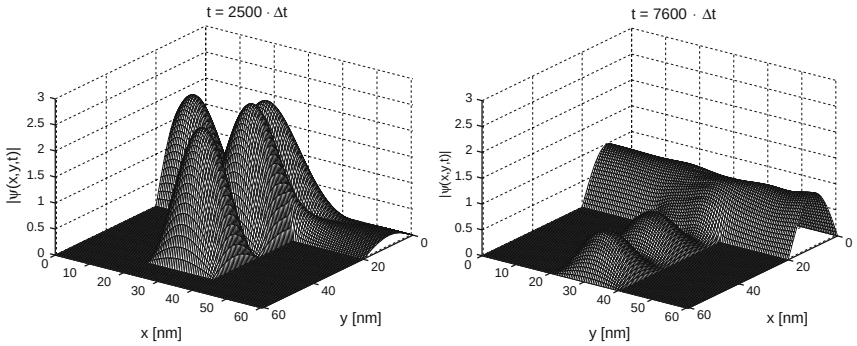

Fig. 2 Stationary Schrödinger wave functions $|\psi(x, y)|$ for a T-shaped waveguide. *Left*: short stub (i.e. $L_1 = 32\,\text{nm}$) – "off state"; *Right*: long stub (i.e. $L_2 = 40.5\,\text{nm}$) – "on state"

to small changes in the applied potential and the geometry, such a device shows sharp peaks in conductance that are due to the presence of trapped charges in the stub (see Fig. 2). It is expected that these novel devices will operate at low power and high speed.

The electron transport through a quantum waveguide can be modeled in good approximation by a two dimensional, time dependent Schrödinger–Poisson system for the (infinitely many) wave functions $\psi_\lambda(x, t)$, indexed by

the energy variable $\lambda \in \Lambda \subset \mathbb{R}$. The (possibly time-dependent) spatial domain $\Omega \subset \mathbb{R}^2$ consists of (very long) leads and the active switching region (e.g. T-shaped as in Fig. 1). In typical applications electrons are constantly fed into the leads as a continuous superposition of plane waves $\psi_\lambda^{pw}(x,t)$, $\lambda \in \Lambda$. Theoretically, $\Lambda = \mathbb{R}$, but for practical simulations it is restricted to a finite interval, and ultimately discretized. The appropriate Schrödinger–Poisson system reads

$$i\hbar \frac{\partial \psi_\lambda}{\partial t} = -\frac{\hbar^2}{2m_*} \Delta \psi_\lambda + eV(x,t)\psi_\lambda, \quad x \in \Omega,\ \lambda \in \Lambda,\ t > 0. \tag{1}$$

Here, $\hbar$ is the reduced Planck constant, m_* the effective electron mass in the semiconductor crystal lattice, and e denotes the (positive) elementary charge. The potential $V = V_e + V_{sc}$ consists of an external, applied potential V_e and the selfconsistent potential satisfying the Poisson equation with Dirichlet boundary conditions:

$$\begin{aligned} -\varepsilon \Delta V_{sc}(x,t) = e\, n(x,t) = e \int_\Lambda |\psi_\lambda(x,t)|^2 g(\lambda)\, d\lambda, \quad x \in \Omega, \\ V_s = 0, \quad \text{on } \partial\Omega. \end{aligned} \tag{2}$$

Here, ε is the permittivity of the semiconductor material and n the spatial electron density. $g(\lambda)$ is a probability distribution, representing the statistics (Fermi–Dirac, e.g.) of the injected waves from both the left and right contact.

In this model we made the following simplifications: We considered only a *single band* and the Schrödinger equation is in the *effective mass approximation*. This means that the effect of the microscopic crystal lattice (yielding a highly oscillatory potential on the atomic length scale) is assumed to be homogenized, and this results in the (constant) effective mass m_*. In heterostructures, however, the effective mass might be space dependent, or even induce nonlocal effects.

This quantum waveguide is connected via leads to an electric circuit. Hence, it is an open system with current flowing through the device. As a consequence, the total electron mass inside the system does not stay constant in time. In typical applications the two leads or contact regions are much longer than suggested by Fig. 1. To reduce computational costs one is therefore obliged to reduce the simulation domain by introducing so-called *open* or *transparent boundary conditions* (TBCs), at $x = 0$ and $x = X$. The purpose of such TBCs is to cut-off the computational domain, but without changing the solution of the original equation. In the simplest case (i.e. a 1D approximation and $V \equiv 0$ in the leads) the TBC takes the form

$$\frac{\partial}{\partial \eta}(\psi_\lambda - \psi_\lambda^{pw}) = -\sqrt{\frac{2m_*}{\hbar}} e^{-i\pi/4} \sqrt{\partial_t}\, (\psi_\lambda - \psi_\lambda^{pw}), \quad \text{for } \lambda \in \Lambda,\ x = 0 \text{ or } x = X, \tag{3}$$

where η denotes the unit outward normal vector at each interface. $\sqrt{\partial_t}$ is the fractional time derivative of order $\frac{1}{2}$, and it can be rewritten as a time-convolution of the boundary data with the kernel $t^{-3/2}$. For the derivation of the 2D-variant of such TBCs and the mathematical analysis of this coupled model (1)–(3) we refer to [BMP05, Arn01, AABES07] and to [LK90] for a stationary Schrödinger-TBC.

To close this subsection we present some simulations of the electron flow through the T-shaped waveguide from Fig. 1 with the dimensions $X = 60\,\mathrm{nm}$, $Y_1 = 20\,\mathrm{nm}$. These calculations are based on the linear Schrödinger equation for a single wave function with $V \equiv 0$ and the injection of a mono-energetic plane wave (i.e. $\Lambda = \{\lambda_0\}$) with $\lambda_0 = 130\,\mathrm{meV}$ from the left lead. The corresponding function $\psi_{\lambda_0}^{pw}(t)$ then appears in formula (3) for the left TBC at $x = 0$. The simulation was based on a compact forth order finite difference scheme ("Numerov scheme") and a Crank–Nicolson discretization in time [AS07, SA07, AJ06].

There are two important device data for practitioners: the current–voltage (I–V) characteristics and the ratio between the on- and the (residual) off-current. This information can be obtained from computing the *stationary Schrödinger states* from the time independent analogue of (1)–(3). Moreover, a third important parameter is the *switching time* between these two stationary states. Depending on the size and shape of the stub, the electron current is either reflected ("off-state" of the device, see Fig. 2, left) or it can flow through the device ("on-state", see Fig. 2, right). In a numerical simulation, this device switching can be realized as follows. Starting from the stationary Schrödinger state shown in Fig. 2 left, we instantaneously extended the stub length from $L_1 = 32\,\mathrm{nm}$ to $L_2 = 40.5\,\mathrm{nm}$. This initiates an evolution of the wave function. After a transient phase of about 4 ps, the new steady state (cf. Fig. 2, right) is reached.

The (complex valued) Schrödinger wave function $\psi(x,t)$, obtained from (1) is rather an auxiliary quantity without intrinsic physical interpretation. Instead, one is rather interested in the following *macroscopic quantities*:

$$n(x,t) := |\psi(x,t)|^2 \ldots \text{ particle density,}$$
$$j(x,t) := \frac{\hbar}{m_*} \Im\left(\bar{\psi}\nabla\psi\right) \ldots \text{ (particle) current density,}$$

which satisfy the *continuity equation*:

$$n_t + \mathrm{div} j = 0\,.$$

If we consider a finite, *closed system* (i.e. without inflow and outflow), mass is preserved in time. In this case one typically has $\psi \in L^2(\mathbb{R}^N;\mathbb{C})$, and frequently chooses the normalization $\int_{\mathbb{R}^N} |\psi(x)|^2 \,\mathrm{d}x = 1$. Then, $\|\psi(\cdot,t)\|_{L^2}^2$ is the (scaled) total mass of the system which is constant under the time evolution by the Schrödinger equation.

Table 1 Examples of the quantization rule

Classical quantity, $a(x,p)$	Quantization, operator A	Expectation value $\langle\psi, A\psi\rangle$
x ... position	x	$\int x\,\lvert\psi\rvert^2\,\mathrm{d}x$
p ... momentum	$-\mathrm{i}\hbar\nabla_x$	$\mathrm{i}\hbar\int\psi\nabla\bar{\psi}\,\mathrm{d}x$
$\frac{\lvert p\rvert^2}{2m}$ ... kinetic energy	$-\frac{\hbar^2}{2m}\Delta_x$	$\frac{\hbar^2}{2m}\int\lvert\nabla\psi\rvert^2\,\mathrm{d}x$
$V(x)$ ... potential (energy)	$V(x)$	$\int V(x)\lvert\psi\rvert^2\,\mathrm{d}x$

As a final remark, we illustrate the relationship between physical variables for classical and quantum particles. Let x and p be, resp., the position and momentum of a classical particle with mass m, and let $a(x,p)$ denote a general physical observable. If that particle is described (at a fixed time) by a classical phase space distribution $f(x,p) \geq 0$ with $(x,p) \in \mathbb{R}^{2N}$ and the typical normalization $\|f\|_{L^1(\mathbb{R}^{2N})} = 1$, the corresponding expectation value of a is

$$\iint_{\mathbb{R}^{2N}} f(x,p)a(x,p)\,\mathrm{d}x\mathrm{d}p\,.$$

For a quantum particle the scalar function $a(x,p)$ is replaced by a (formally) self-adjoint operator A using the *quantization rules* $x \mapsto A := x$ and $p \mapsto A := -\hbar\nabla_x$. Here, $A = x$ denotes the multiplication operator by the variable x. The *expectation value* of the *observable* A in the quantum state ψ is computed as $\langle\psi, A\psi\rangle$ (cf. Table 1 of simple examples).

1.2 Resonant Tunneling Diode

A *resonant tunnel diode* (RTD) is a nano-device which uses quantum effects (tunneling and discrete energy levels) to yield an I–V curve with *negative differential resistance*. Even at room temperature a RTD is capable of generating a tera-Hertz wave, which explains its practical application for ultra high-speed oscillators and possibly for novel digital logic circuits. Presently, RTDs are on the verge of commercialization and extensively studied by engineers.

RTDs have a sandwiched structure of different semiconductor materials (*GaAs* and *AlGaAs*, e.g.) which form two barriers that are only a few nanometers thick (see Fig. 3). This double barrier structure gives rise to a single *quantum well* in its middle. The resulting barrier potential $V_{cont}(x)$ is sketched in Fig. 4. Charge carriers (such as electrons and holes) enter this well by tunneling through a barrier and they can only have particular discrete energy values inside the quantum well. When the energy of the incoming

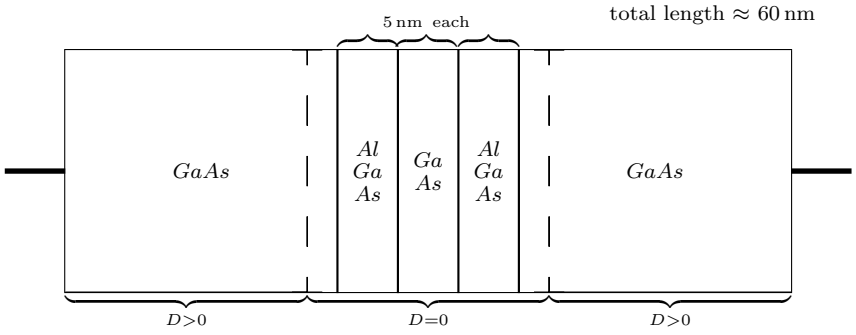

Fig. 3 Schematic 2D cut through a resonant tunneling diode. It consists of the two semiconductor materials $GaAs$ and $AlGaAs$. Close to the two metallic contacts, the crystal lattice is highly doped (with Si, e.g.). $D(x) \geq 0$ is the spatial density of the implanted donor ions

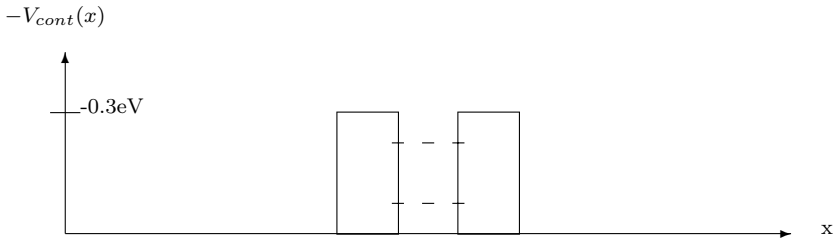

Fig. 4 Effective barrier potential (*contact potential*) V_{cont} for the electron transport induced by the semiconductor heterostructure

electrons coincides with one of these well-energies, their tunneling probability through a barrier rises significantly. Hence, the resulting tunneling current through the double barrier is very peaked at such *resonant energy levels*. In the contact regions of a RTD the crystal lattice is highly doped, i.e. there are donor ions (with Si, e.g.) intentionally implanted into the semiconductor material. Those ions cannot move and their concentration is described by the function $D(x) \geq 0$, the *doping profile*.

A popular and quite accurate simulation model for RTDs is based on Wigner functions [KKFR89, KN06]. Wigner functions are a phase space formulation of quantum mechanics that is equivalent to Schrödinger wave functions (cf. Sect. 5.1 for details). But they seem to be more practical for RTD-simulations, as it is easier to include scattering effects and to formulate (simple) boundary conditions. Their higher dimensionality, however, poses a serious numerical challenge.

The (real valued) Wigner function $w(x, v, t)$ describes the state of a quantum system at time t in the position–velocity phase space. In contrast to

classical phase space probability distributions, w typically takes both positive and negative values. The main macroscopic quantities are obtained as follows:

$$\begin{aligned} n(x,t) &:= \int_{\mathbb{R}^N} w(x,v,t)\,\mathrm{d}v \geq 0 \;\ldots \text{ particle density} \\ j(x,t) &:= \int_{\mathbb{R}^N} v\,w(x,v,t)\,\mathrm{d}v \;\ldots \text{ (particle) current density} \\ e_{kin}(x,t) &:= \frac{m_*}{2}\int_{\mathbb{R}^N} |v|^2 w(x,v,t)\,\mathrm{d}v \geq 0 \;\ldots \text{ kinetic energy density} \end{aligned}$$

Since the Wigner function takes also negative values, it is a-priori not clear why the macroscopic particle density and kinetic energy density should be non-negative, as indicated above. This physically important non-negativity is a consequence of the non-negativity of the density matrix (operator) that is associated with a Wigner function (see Sects. 4.2, 5.1 below).

In order to mathematically formulate a (Wigner function based) quantum transport model of a RTD, we make the following assumptions:

- Only one carrier species is considered: electrons (since the mobility of the holes is too small in such a device to contribute significantly to the charge transport).
- One-particle-like *mean field model* (Hartree approximation).
- Only one parabolic band (with effective mass m_*).
- Purely quantum mechanical transport.
- Ballistics dominates scattering effects (for device lengths up to the order of the electrons' mean free path).

Under the above assumptions, the *Wigner equation* describes the time evolution of the Wigner function w in a given, real valued (electrostatic) potential $V(x,t)$:

$$w_t + v\cdot\nabla_x w - e\,\Theta[V]w = 0, \quad x,v\in\mathbb{R}^N\,. \tag{4}$$

Here, $\Theta[V]$ is a *pseudo-differential operator* (typical abbreviation: "ΨDO"), defined via a multiplication operator for the v-Fourier transformed Wigner function $\mathcal{F}_v w$:

$$\begin{aligned} &\Theta[V]w(x,v) \\ &= \frac{\mathrm{i}}{\hbar}(2\pi)^{-N}\iint_{\mathbb{R}^{2N}}\left[V(x+\frac{\hbar\eta}{2m_*}) - V(x-\frac{\hbar\eta}{2m_*})\right] w(x,\tilde{v})\mathrm{e}^{\mathrm{i}(v-\tilde{v})\cdot\eta}\,\mathrm{d}\tilde{v}\mathrm{d}\eta\,. \end{aligned}$$

Under some regularity and decay assumptions on the potential V, it can be rewritten as convolution operator in v:

$$\Theta[V]w(x,v) \;=\; \alpha(x,v) *_v w(x,v)$$
$$\alpha(x,v) := \frac{2}{\hbar}(2\pi)^{-\frac{N}{2}} \left(\frac{2m_*}{\hbar}\right)^N \Im\left[\mathrm{e}^{\mathrm{i}\frac{2m_*}{\hbar}x\cdot v}\,(\mathcal{F}V)\left(\frac{2m_*}{\hbar}v\right)\right].$$

This convolution form illustrates the non-local effect of potentials in quantum mechanics. Indeed, a particle or wave packet already "feels" an upcoming potential barrier before actually hitting it. Such a "premature" reflection is clearly seen in numerical simulations based on Wigner functions.

For realistic device simulations, scattering (between electrons and impurities or with phonons, i.e. thermal vibrations of the crystal lattice) must be included in the model. Hence, the r.h.s. of (4) has to be augmented by some (at least simple) scattering term. For the 1D simulations of a RTD in [KKFR89] the following relaxation term was used as a phenomenological model for the electron–phonon interactions:

$$w_t + vw_x - e\,\Theta\left[V_{sc}(x,t) + V_{cont}(x)\right] w = \frac{w_{st} - w}{\tau(v)}, \qquad (5)$$
$$0 < x < L,\ v \in \mathbb{R},\ t > 0.$$

Here, w_{st} is some appropriate steady state, and $\tau > 0$ denotes the relaxation time, which may be energy dependent. The spatial interval $(0, L)$ models the diode, and (5) is supplemented by some boundary conditions at the contact points $x = 0$, $x = L$. Motivated by the characteristic lines of the free transport equation $w_t + v \cdot \nabla_x w = 0$, the simplest choice is to prescribe the inflow, i.e. $w^+(0,v)$ for $v > 0$ and $w^-(L,v)$ for $v < 0$ (cf. Fig. 5). This procedure is inspired by classical kinetic theory. The statistical carrier distributions in the two contacts yield the prescribed boundary data $w^+(0,v)$, $w^-(L,v) \geq 0$.

In (5) the potential consists of two contributions: the (time independent) barrier potential $V_{cont}(x)$ and the *self-consistent potential* $V_{sc}(x,t)$, which is due to the mean field approximation. V_{sc} solves the (electrostatic) *Poisson equation*

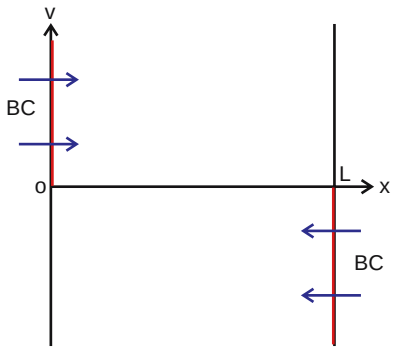

Fig. 5 Vertical slab of x–v-phase space $(0, L) \times \mathbb{R}$ for the 1D Wigner equation: inflow boundary conditions are prescribed at $x = 0$, $v > 0$ and at $x = L$, $v < 0$

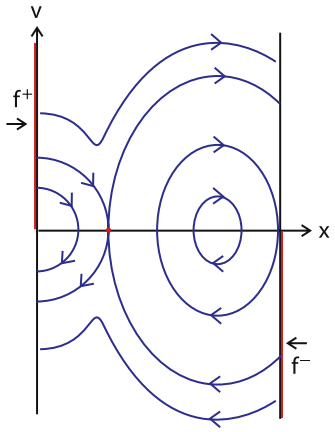

Fig. 6 I–V-characteristics of a RT-diode shows negative differential resistance: (*solid line*) experimental data, (*dashed line*) computed with a simple Schrödinger tunneling model. Reprinted figure with permission from [KKFR89]. Copyright (1989) by the American Physical Society

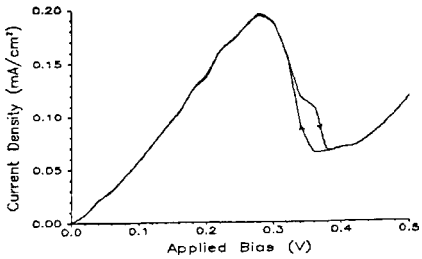

Fig. 7 I–V-characteristics of a RT-diode shows a hysteresis including two stable branches: numerical simulation based on a relaxation-time Wigner–Poisson model. Reprinted figure with permission from [KKFR89]. Copyright (1989) by the American Physical Society

$$\varepsilon \partial_x^2 V_{sc} = e\,(D(x) - n(x,t)), \quad 0 < x < L\,. \tag{6}$$

The non-linear *relaxation-time Wigner–Poisson* model (5)–(6) is used in [KKFR89] for numerical simulations of a RTD. Here, the main goal is to compute the I–V-characteristics and to verify the negative differential resistance of this device. Figures 6 and 7 compare the I–V-curve from experimental data with the numerical results.

For the (semi)classical semiconductor Boltzmann equation excellent models for the most important collisional mechanisms have been derived (cf. [MRS90]) and are incorporated into today's commercial simulation tools. In quantum kinetic theory, however, accurate and numerically usable collision models are much less developed. In contrast to classical kinetic theory, *quantum collision operators* are actually non-local in time (i.e. they include a time integral over the "past", cf. the Levinson equation [Lev70] as one

possible model). However, since most of the existing numerical simulations involve only local in time approximations, we shall confine our discussion to such collision operators Q. The two most used models are the already mentioned relaxation time approximation

$$Qw := \frac{w_{st}(x,v) - w(x,v,t)}{\tau(v)}$$

and the *quantum Fokker–Planck model* with

$$Qw := \underbrace{D_{pp}\Delta_v w}_{\text{class. diffusion}} + \underbrace{2\gamma \operatorname{div}_v(vw)}_{\text{friction}} + \underbrace{D_{qq}\Delta_x w + 2D_{pq}\operatorname{div}_x(\nabla_v w)}_{\text{quantum diffusion}} \tag{7}$$

(cf. [CL83, CEFM00] for a derivation). Both of these models are purely phenomenological, but quantum mechanically "correct" (if $\tau(v) = \tau_0 \geq 0$ or if the *Lindblad condition* (35) holds). And this is important for their mathematical analysis (cf. Sect. 6.2).

As a third option, the r.h.s. of the Wigner equation (4) is often replaced by a semiclassical Boltzmann scattering operator

$$Qw := \int_{\mathbb{R}^N} [S(v,v')w(x,v') - S(v',v)w(x,v)]\, \mathrm{d}v' \,,$$

with the scattering rate $S(v,v')$ (for the electron–phonon interaction, e.g.). Such semiclassical Boltzmann operators give good simulation results [KN06], but they are quantum mechanically *not* "correct" (cf. Sect. 6.1). Hence, we shall not discuss their mathematical analysis.

The RTD-structure is also the key building block of another nano-device, the *resonant tunneling field-effect transistor* (see Fig. 8). This device with three contacts is currently in experimental stage but might become a major building block of logic circuits. It is promising to yield a simple integration of a tunneling diode with the conventional FET structure. Thus it advantageously combines the features of a regular transistor (gain, amplification) with a RTD (negative differential conductance at room temperature). Through an applied gate voltage one can adjust the barrier height, which allows the current peak, the peak-to-valley ratio, and the peak positions to be tuned.

The current from source to drain mainly flows along the channel, which has the same material structure as a RTD (see Fig. 9). Hence, this is also where the quantum effects mainly take place.

These lecture notes are motivated by applicable quantum transport models, which are typically nonlinear partial differential equations (PDEs) on a *bounded domain*, hence, initial boundary value problems (IBVPs). Nevertheless we shall focus the mathematical analysis of quantum evolution problems in the following sections mostly on whole space cases. This is motivated by the fact that much less mathematical analysis has been carried out for those IBVPs. Moreover, these quantum mechanical IBVPs often tend to be much

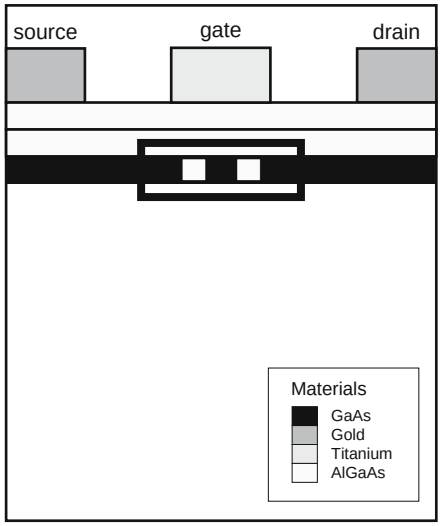

Fig. 8 Schematic 2D cut through a resonant tunneling–FET; dimensions: $0.2\,\mu\mathrm{m}\times 0.2\,\mu\mathrm{m}$. The electron current and quantum effects mainly take place along the channel (*inside the box*)

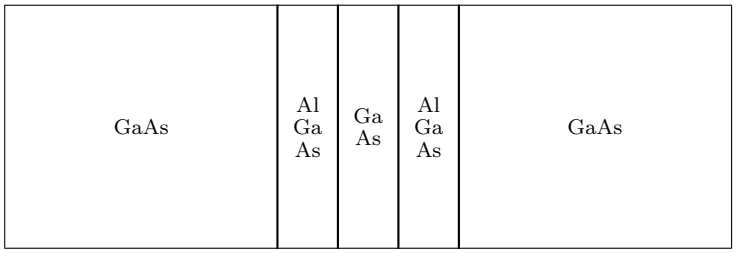

Fig. 9 Enlargement of the central channel region from Fig. 8: There the channel of a is sandwiched structure of the two semiconductor materials *GaAs* and *AlGaAs*

"messier", both from a modeling point of view and mathematically. Consider, as an example, the presented relaxation-time Wigner–Poisson system (an IBVP) for a resonant tunneling diode. With those inflow boundary conditions, it seems impossible to guarantee that the Wigner function $w(t)$ will stay "positive", in the sense of corresponding to a positive density matrix. However, for the corresponding whole space model, this problem does not arise.

2 Linear Schrödinger Equation

In this section we collect some well-known analytical results for the Cauchy problem of the linear Schrödinger equation on $\mathbb{R}^N$. Most of this material is taken from Sect. 3 in [Caz96], and is will serve as our basic background for discussing the nonlinear Schrödinger–Poisson equation in Sect. 3. In these two section we assume that the equations are scaled such that the parameters satisfy $e = m_* = \hbar = 1$.

2.1 Free Schrödinger Group

We consider the *free Schrödinger equation* on $\mathbb{R}^N$ for the complex valued wave function $\psi = \psi(x,t)$:

$$\begin{aligned} \mathrm{i}\psi_t &= -\frac{1}{2}\Delta\psi, \quad t \in \mathbb{R}\,, \\ \psi(0) &= \varphi\,. \end{aligned} \tag{8}$$

The operator $A := \frac{1}{2}\Delta$ with the domain $\mathcal{D}(A) = H^2(R^N)$ is self-adjoint on $L^2(\mathbb{R}^N)$. By Stone's Theorem (cf. [Paz83]) $\mathrm{i}A$ hence generates a C_0-group of isometries on $L^2(\mathbb{R}^N)$:

$$T(t),\ t \in \mathbb{R}; \quad T(t)^* = T(-t)$$

$$T(t_1)T(t_2) = T(t_1{+}t_2), \quad T(0) = I$$

$$\lim_{t\to 0} T(t)\varphi = \varphi \quad \forall \varphi \in L^2(\mathbb{R}^N)$$

$$\lim_{t\to 0} \frac{T(t)\varphi - \varphi}{t} = \mathrm{i}A\varphi \quad \forall \varphi \in \mathcal{D}(A)$$

The operator $\mathrm{i}A$ is call the *infinitesimal generator* of $T(t)$. This evolution group provides a solution to (8) in the following sense:

Proposition 2.1.

(a) Let $\varphi \in L^2(\mathbb{R}^N)$. Then $\psi(t) = T(t)\varphi$ is the unique solution of

$$\begin{cases} \mathrm{i}\psi_t = -\frac{1}{2}\Delta\psi \quad \text{in } H^{-2}(\mathbb{R}^N), \quad \forall t \in \mathbb{R} \\ \psi \in C(\mathbb{R}; L^2(\mathbb{R}^N)) \cap C^1(\mathbb{R}; H^{-2}(\mathbb{R}^N)) \\ \psi(0) = \varphi \end{cases}$$

This mild solution *satisfies mass conservation, i.e. $\|\psi(t)\|_{L^2} = \|\varphi\|_{L^2}$ $\forall t \in \mathbb{R}$ (since $T(t)$ is isometric).*

(b) If $\varphi \in H^2(\mathbb{R}^N)$, the above solution is a classical solution *with $\psi \in C(\mathbb{R}; H^2) \cap C^1(\mathbb{R}; L^2)$.*

Lemma 2.1 (Representation of $T(t)$).

$$T(t)\varphi = K(t) * \varphi \quad \forall t \neq 0,\ \varphi \in \mathcal{S}(\mathbb{R}^N) \tag{9}$$
$$K(x,t) = (8\pi \mathrm{i}t)^{-\frac{N}{2}} \mathrm{e}^{\frac{\mathrm{i}|x|^2}{8t}}$$

Proof. Define $\psi \in C(\mathbb{R}; \mathcal{S}(\mathbb{R}^N))$ by:

$$\hat{\psi}(\xi,t) := \underbrace{\mathrm{e}^{-\frac{\mathrm{i}}{2}|\xi|^2 t}}_{=\hat{K}(\xi,t)} \hat{\varphi}(\xi), \quad \xi \in \mathbb{R}^N \tag{10}$$

$$\Rightarrow \quad \mathrm{i}\hat{\psi}_t = \frac{1}{2}|\xi|^2 \hat{\psi} \quad \text{on } \mathbb{R}_t \times \mathbb{R}^N$$
$$\hat{\psi}(0) = \hat{\varphi}(\xi)$$

□

Note the (formal) similarity between $K(x,t)$, the Green's function of the Schrödinger equation and the heat kernel.

For more regular initial data, the regularity is propagated in time:

Remark 2.1.

(a) Let $\varphi \in H^s(\mathbb{R}^N)$, $s \in \mathbb{R}$. Then $\psi(t) = T(t)\varphi$ satisfies:

$$\psi \in \bigcap_{0 \leq j < \infty} C^j(\mathbb{R}; H^{s-2j}(\mathbb{R}^N)), \qquad \|\psi(t)\|_{H^s} = \|\varphi\|_{H^s}\ .$$

This follows from (10) with $\|\varphi\|_{H^s}^2 = \left\| \left(1+|\xi|^2\right)^{\frac{s}{2}} \hat{\varphi}(\xi) \right\|_{L^2}^2$.

(b)

$$T(t)\varphi = (8\pi \mathrm{i}t)^{-\frac{N}{2}} \mathrm{e}^{\frac{\mathrm{i}|x|^2}{8t}} \int_{\mathbb{R}^N} \mathrm{e}^{-\frac{\mathrm{i}x\cdot y}{4t}} \mathrm{e}^{\frac{\mathrm{i}|y|^2}{8t}} \varphi(y)\,\mathrm{d}y, \quad t \neq 0\,. \tag{11}$$

I.e. $T(t)$ is a Fourier transform up to a rescaling and a multiplication by a function of modulus 1.

2.2 Smoothing Effects and Gain of Integrability in $\mathbb{R}^N$

We shall now discuss simple smoothing properties of the free Schrödinger group $T(t)$. On the one hand we can gain local integrability for $t \neq 0$. On the other hand, (11) shows that $T(t)$, $t \neq 0$ is almost a Fourier transform. And a Fourier transform maps nicely decaying functions into smooth functions. However, the regularity gain for $t \neq 0$ never appears directly on ψ, but it is always coupled to some spatial moments of ψ. This is caused by the multiplier $\mathrm{e}^{\frac{\mathrm{i}|y|^2}{8t}}$ in (11):

Proposition 2.2. *Let the multi-index $\alpha \in \mathbb{N}_0^N$, $\varphi \in \mathcal{S}'(\mathbb{R}^N)$ with $x^\alpha \varphi \in L^2(\mathbb{R}^N)$, and let $\psi(t) = T(t)\varphi \in C(\mathbb{R}; \mathcal{S}'(\mathbb{R}^N))$. Then*

$$\partial_x^\alpha \left(\mathrm{e}^{-\frac{\mathrm{i}|x|^2}{8t}} \psi(t) \right) \in C(\mathbb{R}\backslash\{0\}; L^2(\mathbb{R}^N)),$$

$$(4|t|)^{|\alpha|} \left\| \partial_x^\alpha \left(\mathrm{e}^{-\frac{\mathrm{i}|x|^2}{8t}} \psi(t) \right) \right\|_{L^2} = \|x^\alpha \varphi\|_{L^2}, \quad t \in \mathbb{R}.$$

This follows directly from (11).

Example 2.1. Choose $|\alpha| = 1$:

$$\|(x + 4\mathrm{i}\, t\nabla)\psi(t)\|_{L^2} = \text{const} = \|x\varphi\|_{L^2}, \quad t \in \mathbb{R}.$$

Now we consider the gain of local-in-x integrability:

Proposition 2.3. *Let $2 \le p \le \infty$, $t \neq 0$. Then $T(t) \in \mathcal{B}(L^{p'}(\mathbb{R}^N), L^p(\mathbb{R}^N))$:*

$$\|T(t)\varphi\|_{L^p} \le (8\pi|t|)^{-N\left(\frac{1}{2}-\frac{1}{p}\right)} \|\varphi\|_{L^{p'}} \quad \forall \varphi \in L^{p'}(\mathbb{R}^N). \tag{12}$$

Here and in the sequel $p' = \frac{p}{p-1}$ is the Hölder conjugate of p.

Proof. Let $\varphi \in \mathcal{S}(\mathbb{R}^N)$:

$\|T(t)\varphi\|_{L^\infty} \le (8\pi\|t\|)^{-\frac{N}{2}} \|\varphi\|_{L^1}$	follows from (9) by the Young inequality for convolutions,
$\|T(t)\varphi\|_{L^2} = \|\varphi\|_{L^2}$	since $T(t)$ is isometric.

The result then follows by interpolation (Riesz–Thorin Theorem, [RS75]) and the density of $\mathcal{S}(\mathbb{R}^N)$ in $L^{p'}(\mathbb{R}^N)$. □

2.3 Potentials, Inhomogeneous Equation

Here, we first discuss homogeneous Schrödinger equations with bounded and relatively bounded potentials:

Proposition 2.4 (Bounded perturbations of generators, [Paz83]). *Let A be the infinitesimal generator of the C_0-semigroup $T(t)$ on the Banach space X with $\|T(t)\| \le M\mathrm{e}^{\omega t}$, and $B \in \mathcal{B}(X)$.*

Then $A + B$ generates a C_0-semigroup $S(t)$ on X with

$$\|S(t)\| \le M\mathrm{e}^{(\omega + M\|B\|)t}, \quad t \in \mathbb{R}.$$

Example 2.2. Schrödinger equation with bounded potential $V \in L^\infty(\mathbb{R}^N)$:

$$\begin{cases} \mathrm{i}\psi_t = -\frac{1}{2}\Delta\psi + V\psi, & t \in \mathbb{R} \\ \psi(0) = \varphi \in L^2(\mathbb{R}^N) \end{cases}$$

has a unique mild solution. It is even a classical solution for $\varphi \in H^2(\mathbb{R}^N)$. The *Hamiltonian* of this equation is $H := -\frac{1}{2}\Delta + V$. It reveals conservation of the following energy:

$$\langle \psi(t), H\psi(t)\rangle = \frac{1}{2}\,\|\nabla\psi(t)\|_{L^2}^2 + \int_{\mathbb{R}^N} V n(t)\,\mathrm{d}x = \text{const in } t\,. \tag{13}$$

Next we perturb the free Hamiltonian by a special class of unbounded potentials:

Proposition 2.5 (Relatively bounded perturbations of generators, Kato–Rellich Th. [RS75]). *Let A be a self-adjoint operator on the Hilbert space X, and the operator B symmetric and A-*bounded *(i.e.*

$$\exists a,\, b \in \mathbb{R}:\ \|B\varphi\| < a\|A\varphi\| + b\|\varphi\| \quad \forall \varphi \in \mathcal{D}(A))$$

with $a < 1$. Then $A + B$ is self-adjoint on $\mathcal{D}(A)$.

Example 2.3. Hydrogen atom – motion of one electron in the attractive Coulomb potential of the fixed nucleus:

$$\begin{cases} \mathrm{i}\psi_t = -\frac{1}{2}\Delta\psi - \frac{1}{|x|}\psi, & t \in \mathbb{R} \\ \psi(0) = \varphi \in L^2(\mathbb{R}^3) & (\text{or } \varphi \in H^2(\mathbb{R}^3)) \end{cases}$$

has a unique mild (or, resp., classical) solution. To prove this, we split the potential $V(x) = \frac{1}{|x|}$ into a short and long range potential:

$$V = V_1 + V_2 \quad \text{with}$$

$$V_1 \in L^2(\mathbb{R}^3),\ V_2 := \min\left(1, \frac{1}{|x|}\right) \in L^\infty(\mathbb{R}^3)\,.$$

V_1 is Δ-bounded because of $\psi \in H^2(\mathbb{R}^3) \hookrightarrow L^\infty(\mathbb{R}^3)$ by a Sobolev embedding. Hence, Proposition 2.5 applies to V_1 and Proposition 2.4 applies to V_2.

Now we turn to inhomogeneous Schrödinger equations:

Proposition 2.6. *Let $\varphi \in L^2(\mathbb{R}^N)$, $f \in C([0,T]; L^2(\mathbb{R}^N))$.*

(a) Then $\exists!$ solution of

$$\begin{cases} \mathrm{i}\psi_t + \frac{1}{2}\Delta\psi + f = 0 \quad \forall t \in [0,T] \\ \psi \in C([0,T]; L^2(\mathbb{R}^N)) \cap C^1([0,T]; H^{-2}(\mathbb{R}^N)) \\ \psi(0) = \varphi\,. \end{cases}$$

With $T(t)$ denoting the free Schrödinger group, this mild solution *satisfies*

$$\psi(t) = T(t)\varphi + \mathrm{i}\int_0^t T(t-s)f(s)\,\mathrm{d}s, \quad 0 \le t \le T. \tag{14}$$

(b) Let, additionally, $\varphi \in H^2(\mathbb{R}^N)$ and either $f \in W^{1,1}((0,T);L^2(\mathbb{R}^N))$ or $f \in L^1((0,T);H^2(\mathbb{R}^N))$. Then ψ is a (classical solution)*, satisfying $\psi \in C(\mathbb{R};H^2) \cap C^1(\mathbb{R};L^2)$.*

2.4 Strichartz Estimates

The goal of this subsection is to derive combined space–time estimates for the inhomogeneous Schrödinger equation (14).

Definition 2.1. A pair of indices (q,p) is called *admissible* if

$$2 \le p < \tfrac{2N}{N-2} \quad (\text{or } 2 \le p \le \infty \text{ if } N=1;\ 2 \le p < \infty \text{ if } N=2),$$
$$\tfrac{2}{q} = N\left(\tfrac{1}{2} - \tfrac{1}{p}\right).$$

Notation:

$$L^{q,p} := L^q(\mathbb{R}_t; L^p(\mathbb{R}^N))$$
$$L_I^{q,p} := L^q(I; L^p(\mathbb{R}^N)) \quad \text{for any interval } I \subset \mathbb{R}$$

The following *Strichartz estimate* for the free and inhomogeneous Schrödinger equation describes a gain of local-in-x integrability. Since the following inequalities hold in a mixed space-time norm, this gain of integrability does not hold pointwise in time, but for almost all t:

Proposition 2.7. *Let (q,p), (a,b) be admissible pairs.*

(a) Let $\varphi \in L^2(\mathbb{R}^N)$. Then $T(t)\varphi \in L^{q,p} \cap C(\mathbb{R};L^2(\mathbb{R}^N))$ with

$$\|T(\cdot)\varphi\|_{L^{q,p}} \le C(q)\|\varphi\|_{L^2}. \tag{15}$$

(b) Let $f \in L_I^{a',b'}$ and $t_0 \in \bar{I}$. Then it holds

$$\Lambda_f(t) := \int_{t_0}^t T(t-s)f(s)\,\mathrm{d}s \in L_I^{q,p} \cap C(\bar{I};L^2(\mathbb{R}^N))$$

with

$$\|\Lambda_f\|_{L_I^{q,p}} \le C(a,q)\|f\|_{L_I^{a',b'}}.$$

The constants $C(q)$ and $C(a,q)$ are independent of time.

Proof (of the inhomogeneous version for $(a,b) = (q,p)$. The general case depends on duality arguments, see Sect. 3.2 of [Caz96]).

Let $I = [0,T]$, $t_0 = 0$, $f \in C_0([0,T]; L^{p'})$; the result for general $f \in L^{q,p}$ then follows by density. Inequality (12) and $N(\frac{1}{2} - \frac{1}{p}) = \frac{2}{q}$ yield:

$$\|\Lambda_f(t)\|_{L^p} \le C(q) \int_0^t |t-s|^{-N(\frac{1}{2}-\frac{1}{p})} \|f(s)\|_{L^{p'}} \, \mathrm{d}s$$

$$\le C(p) \int_0^T |t-s|^{-\frac{2}{q}} \|f(s)\|_{L^{p'}} \, \mathrm{d}s \, .$$

With the weak Young inequality (cf. [RS75]) we conclude:

$$\|\Lambda_f\|_{L_I^{q,p}} \le C(q) \|f\|_{L_I^{q',p'}} \, .$$

□

Remark 2.2.

(a) In Proposition 2.7a $\varphi \in L^2(\mathbb{R}^N)$ implies $T(t)\varphi \in L^p$ for almost all $t \in \mathbb{R}$ (for $p > 2$). It cannot be improved to "for all $t \neq 0$".

(b) Since the Schrödinger equation is time reversible, the presented smoothing effects are much more subtle than for the heat equation. The evolution also improves the local integrability of the solution ψ for almost all t. The smoothing effects in Propositions 2.3 and 2.7 are due to the dispersion *in the Schrödinger equation. This means that waves of different frequencies (or wavelengths) travel at different velocities, when decomposing the solution ψ into plane waves.*

(c) A remarkable aspect of Proposition 2.7b is that the index pairs (q,p) and (a',b') are uncorrelated.

3 Schrödinger–Poisson Analysis in $\mathbb{R}^3$

The goal of this section is to prove that the repulsive Schrödinger–Poisson (SP) equation (or *Hartree equation*) in $\mathbb{R}^3$ has a unique, global-in-time solution, first for initial data in H^1 and then in L^2. We shall mostly follow Sect. 6.3 of [Caz96] and [Cas97]; but see also [GV94, HO89]. We remark that extensions of this analysis to the Sobolev spaces H^k, $k \ge 2$ is straightforward [Caz96]. Extensions to space dimensions $N \neq 3$ require some modifications, since the used Sobolev embeddings depend on N [Caz96, AN91].

3.1 H^1-Analysis

A wave function $\psi \in H^1$ corresponds to a system with *finite mass* $\|\psi\|_{L^2}^2$ and *finite kinetic energy* $\frac{1}{2}\|\nabla\psi\|_{L^2}^2$. As we shall see, this property is propagated in time.

In the sequel we shall frequently need the following result on solutions to nonlinear Banach space-ODEs (i.e. an ordinary differential equation for a Banach space-valued function):

Proposition 3.1 (Local Lipschitz perturbations of generators [Paz83]). *Let A be the infinitesimal generator of the C_0-semigroup $T(t)$, $t \geq 0$ on the Banach space X, and let $f = f(t,u) : [0,\infty) \times X \to X$ be continuous in t and locally Lipschitz in u (uniformly in t on bounded intervals).*

(a) Then, $\forall \varphi \in X$, $\exists t_{max} = t_{max}(\varphi) \leq \infty$:

$$\begin{cases} \frac{\mathrm{d}u}{\mathrm{d}t} = Au + f(t,u(t)), & t \geq 0 \\ u(0) = \varphi \end{cases}$$

has a unique mild solution $u \in C([0,t_{max}); X)$.
(b) If $t_{max} < \infty$ then $\lim_{t \nearrow t_{max}} \|u(t)\|_X = \infty$, i.e. blow-up in finite time.
(b′) If $\|u(t)\|_X < \infty \ \forall t \in [0,\infty) \ \Rightarrow$ The solution exists global-in-time.

This theorem will now be applied to the repulsive *Schrödinger–Poisson* equation (or *Hartree equation*):

$$\begin{cases} \mathrm{i}\psi_t = -\frac{1}{2}\Delta\psi + V\psi, & x \in \mathbb{R}^3,\ t \in \mathbb{R} \\ -\Delta_x V(x,t) = n(x,t) := |\psi(x,t)|^2 \\ \psi(0) = \varphi \end{cases} \tag{16}$$

We take the *Newton potential solution* of the Poisson equation:

$$\begin{aligned} V &= \tfrac{1}{4\pi|x|} * |\psi|^2 \\ \nabla V &= -\tfrac{x}{4\pi|x|^3} * |\psi|^2 \end{aligned} \tag{17}$$

Theorem 3.1. *Let $\varphi \in H^1(\mathbb{R}^3)$. Then* (16) *has a unique solution $\psi \in C(\mathbb{R}; H^1(\mathbb{R}^3))$.*

Proof.

1. $T(t) = e^{\frac{\mathrm{i}}{2}\Delta t}$ is a C_0-group of isometries both on $L^2(\mathbb{R}^3)$ and $H^1(\mathbb{R}^3)$.
2. $f(\psi) := -\mathrm{i}V[\psi]\psi = -\mathrm{i}\left(\frac{1}{4\pi|x|} * |\psi|^2\right)\psi$ is locally Lipschitz in H^1 (but *not* in L^2; hence we analyze (16) in H^1) since:
   The weak Young inequality (cf. [RS75]) for (17) yields:

$$\begin{aligned} \|V\|_{L^p} &\leq C\|\psi\|_{L^q}^2, \qquad 3 < p \leq \infty, \quad \tfrac{1}{p} = \tfrac{2}{q} - \tfrac{2}{3}\,, \\ \|\nabla V\|_{L^p} &\leq C\|\psi\|_{L^q}^2, \qquad \tfrac{2}{3} < p < \infty, \quad \tfrac{1}{p} = \tfrac{2}{q} - \tfrac{1}{3}\,, \end{aligned} \tag{18}$$

and Hölder's inequality and the Sobolev embedding $H^1(\mathbb{R}^3) \hookrightarrow L^6(\mathbb{R}^3)$ yield:

$$\begin{aligned} \|f(\psi)\|_{L^2} &\le \|V\|_{L^\infty}\|\psi\|_{L^2} \le C\|\psi\|_{H^1}^3 , \\ \|\nabla f(\psi)\|_{L^2} &\le \|V\|_{L^\infty}\|\nabla\psi\|_{L^2} + \|\nabla V\|_{L^3}\|\psi\|_{L^6} \le C\|\psi\|_{H^1}^3 . \end{aligned}$$

3. By Proposition 3.1 it holds: The Schrödinger–Poisson equation (16) has a *unique local solution* $\psi \in C([0,t_{max}); H^1(\mathbb{R}^3))$.
4. $\|\psi\|_{H^1}$ cannot blow up in finite time because of the following two estimates:
   (a) L^2 *– a priori estimate (mass conservation):*
   The Schrödinger equation (16) holds in $C([0,t_{max}); H^{-1})$. We test it against $\psi(t) \in H^1$:
   $$\mathrm{i}\langle\psi_t,\psi\rangle = \frac{1}{2}\|\nabla\psi\|_{L^2}^2 + \int_{\mathbb{R}^3} V|\psi|^2 \,\mathrm{d}x .$$
   Taking the imaginary part yields: $\frac{\mathrm{d}}{\mathrm{d}t}\|\psi\|_{L^2}^2 = 0$.
   (b) $\dot{H}^1$ *– a priori estimate (energy conservation):*
   We test the Schrödinger equation (16) against ψ_t and integrate by parts. A formal calculation yields:
   $$\mathrm{i}\|\psi_t\|_{L^2}^2 = \frac{1}{2}\int_{\mathbb{R}^3} \nabla\psi\cdot\nabla\bar{\psi}_t \,\mathrm{d}x + \int_{\mathbb{R}^3} V\psi\bar{\psi}_t \,\mathrm{d}x .$$
   Taking the real part and using the Poisson equation yield:
   $$\begin{aligned} 0 &= \tfrac{1}{2}\tfrac{\mathrm{d}}{\mathrm{d}t}\|\nabla\psi\|_{L^2}^2 + \textstyle\int_{\mathbb{R}^3} V n_t \,\mathrm{d}x = \tfrac{1}{2}\tfrac{\mathrm{d}}{\mathrm{d}t}\|\nabla\psi\|_{L^2}^2 + \textstyle\int_{\mathbb{R}^3} \nabla V\cdot\nabla V_t \,\mathrm{d}x \\ &= \tfrac{\mathrm{d}}{\mathrm{d}t}\Big[\underbrace{\frac{1}{2}\|\nabla\psi(t)\|_{L^2}^2}_{\text{kinetic energy}} + \underbrace{\frac{1}{2}\|\nabla V(t)\|_{L^2}^2}_{\text{self-consist. potential energy}} \Big] \end{aligned}$$
   Hence, $\|\nabla\psi(t)\|_{L^2}$ is uniformly bounded in t.

   Remark: Here, the (self-consistent) potential energy is $\frac{1}{2}\|\nabla V\|_{L^2}^2 = \frac{1}{2}\int Vn \,\mathrm{d}x$, while it is $\int Vn \,\mathrm{d}x$ in the linear case (cf. (13)).
5. $\Rightarrow$ The solution exists $\forall t \in \mathbb{R}$. □

3.2 L^2-Analysis

If a wave function $\psi \in L^2$ but *not* in H^1, the corresponding quantum system has *finite mass* but *infinite kinetic energy*.

Since the nonlinearity $f(\psi) := -\mathrm{i}V[\psi]\psi = -\mathrm{i}\left(\frac{1}{4\pi|x|} * |\psi|^2\right)\psi$ is *not* locally Lipschitz in L^2, our analysis is much more difficult than the H^1-analysis above. Here we shall use that $f(\psi)$ is still (somehow) locally Lipschitz in the following space of t-dependent functions: $L_T^{q,p} := L^q((-T,T);L^p(\mathbb{R}^3))$, for some fixed $T > 0$.

We split the self-consistent potential $V[\psi]$ into a short and a long range potential: $V[\psi] = V_1[\psi] + V_2[\psi]$, with $V_2[\psi] := \frac{1}{4\pi}\min(1, \frac{1}{|x|}) * |\psi|^2$. And we split the nonlinearity $f(\psi)$ analogously: $f(\psi) = f_1(\psi) + f_2(\psi)$, with $f_j(\psi) := -iV_j[\psi]\psi$.

The following result shows that $f_{1,2}(\psi)$ are locally Lipschitz, however, in different spaces $L_T^{q,p}$.

Lemma 3.1 ([Cas97]). *Let $0 < T < 1$; $3 < p < 6$; $q = q(p)$ with $\frac{2}{q} = 3(\frac{1}{2} - \frac{1}{p})$; ψ, $\phi \in C([-T,T];L^2(\mathbb{R}^3)) \cap L_T^{q,p}$; $M := \max_{[-T,T]}(\|\psi(t)\|_{L^2}, \|\phi(t)\|_{L^2})$. Then*

(a)

$$\|f_1(\psi(t)) - f_1(\phi(t))\|_{L_T^{q',p'}} \le C(p)M^2T^{1-\frac{2}{q}}\|\psi(t) - \phi(t)\|_{L_T^{q,p}},$$

(b)

$$\begin{aligned}\|f_2(\psi(t)) - f_2(\phi(t))\|_{L_T^{1,2}} &\le CM^2T\|\psi(t) - \phi(t)\|_{L_T^{\infty,2}} \\ &\le CM^2T^{1-\frac{2}{q}}\|\psi(t) - \phi(t)\|_{L_T^{\infty,2}}.\end{aligned}$$

Theorem 3.2. *Let $\varphi \in L^2(\mathbb{R}^3)$. Then the Schrödinger–Poisson equation* (16) *has a unique mild solution $\psi \in C(\mathbb{R};L^2(\mathbb{R}^3)) \cap L_{loc}^{q,p}$ with $3 < p < 6$, $\frac{2}{q} = 3(\frac{1}{2} - \frac{1}{p})$.*

Proof.

1. *Approximating H^1-sequence to construct a solution:*
   Let $\{\varphi_m\}_{m\in\mathbb{N}} \subset H^1(\mathbb{R}^3)$ with $\varphi_m \overset{m\to\infty}{\longrightarrow} \varphi$ in L^2, $\|\varphi_m\|_{L^2} = \|\varphi\|_{L^2}$.
   By Theorem 3.1, for each φ_m, $m \in \mathbb{N}$, the SP-problem then has a unique solution $\psi_m \in C(\mathbb{R};H^1(R^3))$, satisfying $\|\psi_m(t)\|_{L^2} = \|\varphi\|_{L^2} =: M$ $\forall t \in \mathbb{R}$.
2. *$\{\psi_m(t)\}$ is a Cauchy sequence in $L_T^{a,b}$ for T small:*

$$\begin{aligned}\psi_m(t) - \psi_k(t) &= T(t)(\varphi_m - \varphi_k) \\ &\quad + \textstyle\int_0^t T(t-s)[f_1(\psi_m(s)) - f_1(\psi_k(s))]\,\mathrm{d}s \\ &\quad + \textstyle\int_0^t T(t-s)[f_2(\psi_m(s)) - f_2(\psi_k(s))]\,\mathrm{d}s\end{aligned} \tag{19}$$

The homogeneous Strichartz inequality (Proposition 2.7a) yields:

$$\|T(t)(\varphi_m - \varphi_k)\|_{L_T^{a,b}} \le C(a)\|\varphi_m - \varphi_k\|_{L^2}.$$

The inhomogeneous Strichartz inequality (Proposition 2.7b) and Lemma 3.1a yield for the first nonlinearity:

$$\begin{aligned}\| \int_0^t T(t-s)[f_1(\psi_m(s)) - f_1(\psi_k(s))]\, ds\|_{L_T^{a,b}} \\ &\leq C(a,q)\|f_1(\psi_m(t)) - f_1(\psi_k(t))\|_{L_T^{q',p'}} \\ &\leq C(a,q)M^2T^{1-\frac{2}{q}}\|\psi_m(t) - \psi_k(t)\|_{L_T^{q,p}}\,.\end{aligned}$$

Here, (a,b) is any admissible pair.
Similarly, the inhomogeneous Strichartz inequality (Proposition 2.7b) and Lemma 3.1b yield for the second nonlinearity:

$$\begin{aligned}\| \int_0^t T(t-s)[f_2(\psi_m(s)) - f_2(\psi_k(s))]\, \mathrm{d}s\|_{L_T^{a,b}} \\ &\leq C(a)M^2T^{1-\frac{2}{q}}\|\psi_m(t) - \psi_k(t)\|_{L_T^{\infty,2}}\end{aligned}$$

We collect the last three inequalities and add the resulting estimates for the two index-choices $(a,b) = (q,p)$, $(a,b) = (\infty,2)$. This yields the following estimate for (19):

$$\begin{aligned}&\|\psi_m(t) - \psi_k(t)\|_{L_T^{q,p}} + \|\psi_m(t) - \psi_k(t)\|_{L_T^{\infty,2}} \\ &\quad\leq C(q)\|\varphi_m - \varphi_k\|_{L^2} \\ &\qquad +C(q)M^2T^{1-\frac{2}{q}}\left[\|\psi_m(t) - \psi_k(t)\|_{L_T^{q,p}} + \|\psi_m(t) - \psi_k(t)\|_{L_T^{\infty,2}}\right]\end{aligned}$$

$\Rightarrow\ \exists\, T_0 = T_0(q,M) > 0$, small enough such that:

$$\|\psi_m(t)-\psi_k(t)\|_{L_{T_0}^{q,p}}+\|\psi_m(t)-\psi_k(t)\|_{L_{T_0}^{\infty,2}} \leq C(q,M)\|\varphi_m-\varphi_k\|_{L^2}\,. \quad (20)$$

This implies the following properties of the approximating sequence $\{\psi_m\}$:

- $\{\psi_m\}$ is a Cauchy sequence in $L_{T_0}^{q,p} \cap L_{T_0}^{\infty,2}$.
- $\{\psi_m\} \subset C([-T_0,T_0]; L^2(\mathbb{R}^3))$.
- $\psi_m \to \psi$ in $L_{T_0}^{q,p} \cap C([-T_0,T_0]; L^2(\mathbb{R}^3))$.
- $\|\psi_m(t)\|_{L^2} = \|\psi(t)\|_{L^2} = \|\varphi\|_{L^2} = M, \quad \forall\, m \in \mathbb{N},\, \forall t \in \mathbb{R}\,.$

Since $T_0 = T_0(q,M)$ only depends on the index q and $M = \|\varphi\|_{L^2}$, the solution ψ can be extended up to $2T_0$, $3T_0$, ..., $-T_0$, $-2T_0$, ... Hence, $\psi \in C(\mathbb{R}; L^2(\mathbb{R}^3)) \cap L_{loc}^{q,p}$.
The estimate (20) also implies uniqueness of the limit ψ and its continuous dependence on the data φ. The constructed limit ψ is the mild solution of (16). To verify this, choose $\psi_k := 0$ and pass to the limit ($m \to \infty$) in the integral equation (19). □

3.3 Schrödinger–Poisson Systems

Up to now we considered just one Schrödinger equation that is coupled to the Poisson equation. This would describe a *pure quantum state*. In most realistic application, however, one has to deal with a *mixed quantum state*, which can be described by a sequence of wave functions:

$$\psi_j(x,t) \in \mathbb{C},\ j \in \mathbb{N};\ x \in \mathbb{R}^3,\ t \in \mathbb{R}\,.$$

For a system of many particles, this mixed quantum state describes a statistical mixture, and each ψ_j has an *occupation probability* $\lambda_j \geq 0$, $j \in \mathbb{N}$; $\sum_j \lambda_j = 1$. Here, λ_j are given data and it depends on the initial state of the system.

In this section we only consider *closed quantum systems*, i.e. a system without interaction to an (infinitely large) "environment" or "heat bath". Its dynamics is time-reversible and fully described by a Hamiltonian. In this case the above occupation probabilities λ_j are constant in time.

Open quantum systems, being the opposite of closed quantum systems will be discussed in Sect. 6.

We consider now the time evolution of this mixed quantum state, given by the *repulsive Schrödinger–Poisson system* (SPS):

$$\begin{cases} \mathrm{i}\frac{\partial}{\partial t}\psi_j = -\frac{1}{2}\Delta\psi_j + V\psi_j, & x \in \mathbb{R}^3,\ t \in \mathbb{R},\ j \in \mathbb{N} \\ V(x,t) = \frac{1}{4\pi|x|} * n(x,t), & n(x,t) := \sum_{j=1}^{\infty} \lambda_j |\psi_j(x,t)|^2 \\ \psi_j(0) = \varphi_j, & j \in \mathbb{N} \end{cases} \tag{21}$$

In the special case $\lambda_j := \delta_j^1$ (δ_j^i is the Kronecker-Delta) the SPS reduces to the scalar Hartree equation of Sect. 3.1. In the subsequent analysis we follow mostly [Cas97].

Notation:
For any fixed sequence $\lambda := \{\lambda_j\}_{j\in\mathbb{N}} \in \ell^1$ with $\lambda_j \geq 0$ we define:

$$\begin{aligned} H^1(\lambda) &:= \{\Phi(x) = (\varphi_j(x))_{j\in\mathbb{N}},\ \|\Phi\|^2_{H^1(\lambda)} = \textstyle\sum_j \lambda_j \|\varphi_j(x)\|^2_{H^1(\mathbb{R}^3)} < \infty\} \\ L^p(\lambda) &:= \{\Phi(x) = (\varphi_j(x))_{j\in\mathbb{N}},\ \|\Phi\|^2_{L^p(\lambda)} = \textstyle\sum_j \lambda_j \|\varphi_j(x)\|^2_{L^p(\mathbb{R}^3)} < \infty\} \\ L^{q,p}_{loc}(\lambda) &:= L^q_{loc}(\mathbb{R}; L^p(\lambda)) \end{aligned}$$

Theorem 3.3.

(a) Let $\Phi \in H^1(\lambda)$. Then (21) *has a unique solution $\Psi \in C(\mathbb{R}; H^1(\lambda))$.*
(b) [Cas97]: Let $\Phi \in L^2(\lambda)$. Then (21) *has a unique mild solution $\Psi \in C(\mathbb{R}; L^2(\lambda) \cap L^{q,p}_{loc}(\lambda))$ for all admissible pairs (q,p) with $3 < p < 6$, $\frac{2}{q} = 3(\frac{1}{2} - \frac{1}{p})$.*

Proof.

(a) This is a straightforward generalization of Theorem 3.1 for the Hartree equation (cf. [ILZ94], e.g.):
$f(\Psi) := -\mathrm{i}V[\Psi]\Psi$ is locally Lipschitz in $H^1(\lambda)$. The required a-priori estimates are provided by $\|\Psi(t)\|^2_{L^2(\lambda)} = \|\Phi\|^2_{L^2(\lambda)}$ (mass conservation) and $\frac{1}{2}\|\nabla\Psi(t)\|^2_{L^2(\lambda)} + \frac{1}{2}\|\nabla V(t)\|^2_{L^2} = \text{const.}$ (energy conservation).

(b) This part is based on *vector valued Strichartz inequalities* for mixed quantum states which are non-trivial extensions of Proposition 2.7. E.g., the extension of the homogeneous estimate (15) reads ([Cas97]):

$$\|T(t)\Phi\|_{L^{q,p}_T(\lambda)} \le C(q,T)\|\Phi\|_{L^2(\lambda)} \quad \forall \text{ admissible pairs } (q,p)$$

with

$$\|T(t)\Phi\|^q_{L^{q,p}_T(\lambda)} = \int_{-T}^{T} \Big(\sum_j \lambda_j \|T(t)\varphi_j\|^2_{L^p}\Big)^{\frac{q}{2}} \mathrm{d}t.$$

In contrast, a trivial extension of Proposition 2.7 would be

$$\sum_j \lambda_j \|T(t)\varphi_j\|^2_{L^{q,p}} \le C(q) \sum_j \lambda_j \|\varphi_j\|^2_{L^2},$$

but it is not useful here.

□

4 Density Matrices

In this section we present an alternative description of mixed quantum states which is (formally) equivalent to the Schrödinger system of Sect. 3.3 (see [AF01, DL88, DL88a] for more details).

4.1 Framework, Trace Class Operators

Let $\mathcal{J}_1(L^2(\mathbb{R}^N))$ denote the Banach space of trace class operators on $L^2(\mathbb{R}^N)$, and $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^N))$ its closed subspace of self-adjoint operators.

Definition 4.1. A *density matrix (operator)* is a positive, self-adjoint trace class operator on $L^2(\mathbb{R}^N)$, i.e. $\hat{\varrho} \in \tilde{\mathcal{J}}_1(L^2(\mathbb{R}^N))$ with $\hat{\varrho} \ge 0$.

Since $\hat{\varrho}$ is self-adjoint and compact, there exists a complete ONS $\{\psi_j\}_{j\in\mathbb{N}} \subset L^2(\mathbb{R}^N)$ of eigenvectors. Since $\hat{\varrho}$ is positive and trace class, its eigenvalues satisfy $\lambda_j \ge 0$, $\{\lambda_j\}_{j\in\mathbb{N}} \subset \ell^1$.

We remark that the eigenvectors ψ_j are exactly the pure state wave functions from Sect. 3.3, and the eigenvalues λ_j are the their occupation probabilities.

A typical normalization (on the total mass) is: $\operatorname{Tr}\hat{\varrho} = \sum_j \lambda_j = 1$. The norm of a self-adjoint (but non necessarily positive) trace class operators is given by:

$$\|\!|\hat{\varrho}|\!\|_1 := \operatorname{Tr}|\hat{\varrho}| \overset{\hat{\varrho}\text{ s.a.}}{=} \sum_j |\lambda_j| \,.$$

Each density matrix operator has a unique integral representation:

$$(\hat{\varrho}f)(x) = \int_{\mathbb{R}^N} \varrho(x,y) f(y)\,\mathrm{d}y \qquad \forall f \in L^2(\mathbb{R}^N)$$

with the *density matrix function*

$$\varrho(x,y) = \sum_j \lambda_j \psi_j(x)\bar{\psi}_j(y) \in L^2(\mathbb{R}^{2N}) \,. \tag{22}$$

Here, $x, y \in \mathbb{R}^N$ are position variables. The self-adjointness of $\hat{\varrho}$ implies $\bar{\varrho}(x,y) = \varrho(y,x)$.

The L^2-norm of ϱ and the Hilbert–Schmidt norm $\|\!|\hat{\varrho}|\!\|_2$ of $\hat{\varrho}$ are related by

$$\|\varrho\|_2 = \|\!|\hat{\varrho}|\!\|_2 := (\operatorname{Tr}|\hat{\varrho}|^2)^{\frac{1}{2}} \le \|\!|\hat{\varrho}|\!\|_1 \,.$$

4.2 Macroscopic Quantities

We shall now define the most important macroscopic quantities of a quantum state that is modeled by a density matrix. We give two parallel definitions, both when the system is described by a density matrix *function* and a density matrix *operator*.

(a) Definition from the integral kernel $\varrho(x,y)$: The following formulae can be obtained from the analogous expressions for a wave function (see Sect. 1.1) and the eigenfunction expansion (22).

Particle density:
For $0 \le \hat{\varrho} \in \tilde{\mathcal{J}}_1$ it holds:

$$\begin{aligned} &n(x) := \varrho(x,x) = \textstyle\sum_j \lambda_j |\psi_j(x)|^2 \in L^1\left(\mathbb{R}^N\right), \quad n(x) \ge 0 \text{ since } \lambda_j \ge 0 \,, \\ &\|n\|_{L^1(\mathbb{R}^N)} \le \textstyle\sum_j |\lambda_j| \, \|\psi_j\|_{L^2}^2 = \|\!|\hat{\varrho}|\!\|_1 \overset{\hat{\varrho}\ge 0}{=} \operatorname{Tr}\hat{\varrho} \,. \end{aligned} \tag{23}$$

Remark 4.1. *While $n(x)$ is defined a.e. for $\hat{\varrho} \in \mathcal{J}_1$, the definition* $n(x) := \varrho(x,x)$ is meaningless *for Hilbert–Schmidt operators $\hat{\varrho} \in \mathcal{J}_2$. Moreover, then there is no natural estimate of n in terms of the density matrix function ϱ.*

This leads to the following problem for an evolution equation of $\hat{\varrho}$: For an operator $\hat{\varrho} \in \mathcal{J}_2$ there is a simple functional representation of the corresponding integral kernel: $\hat{\varrho} \in \mathcal{J}_2(L^2) \Leftrightarrow \varrho \in L^2(\mathbb{R}^{2N})$, but for $\hat{\varrho} \in \mathcal{J}_1$ no *'nice' equivalent space exists for the kernel $\varrho(x,y)$. Now, if one wants to describe the time evolution of a density matrix $\hat{\varrho} \in \mathcal{J}_2(L^2(\mathbb{R}^N))$, a PDE for $\varrho \in L^2(\mathbb{R}^{2N})$ is the natural choice (see* (27)*, below). However, in this framework the particle density $n(x)$ cannot be defined. For a self-consistent model we therefore need to consider the time evolution of a density matrix $\hat{\varrho} \in \mathcal{J}_1(L^2(\mathbb{R}^N))$. Due to the lack of a corresponding function space for its kernel, this must be considered as abstract evolution problem (Banach space–ODE) for $\hat{\varrho}(t) \in \mathcal{J}_1$ (see* (28)*, below) instead of a PDE for its kernel $\varrho(t)$!*

Higher order macroscopic quantities are formally defined as:
Current density:

$$j(x) := \Im \nabla_x \varrho\Big|_{x=y} = \sum_j \lambda_j \Im[\nabla\psi_j(x)\bar{\psi}_j(x)]\,.$$

Kinetic energy density:

$$e_{kin}(x) := \frac{1}{2}(\nabla_x \cdot \nabla_y)\varrho\Big|_{x=y} = \frac{1}{2}\sum_j \lambda_j |\nabla\psi_j(x)|^2 \geq 0 \quad \text{since } \lambda_j \geq 0\,.$$

(b) Definition from the trace class operator $\hat{\varrho} \in \mathcal{J}_1$:

Particle density:
$n[\hat{\varrho}]$ can be defined by duality as

$$\int \varphi(x) n(x)\,\mathrm{d}x = \mathrm{Tr}\,(\varphi\ \hat{\varrho}) = \mathrm{Tr}\,(\hat{\varrho}\ \varphi) \qquad \forall \varphi \in L^\infty(\mathbb{R}^N)\,, \tag{24}$$

where φ inside the operator trace Tr means the bounded multiplication operator by the function $\varphi \in L^\infty$. If (24) holds $\forall \varphi \in C_0(\mathbb{R}^N)$, n is defined as a *Radon measure* on $\mathbb{R}^N$ (cf. [Bre87]).
Kinetic energy:
A formal calculation shows

$$E_{kin}(\hat{\varrho}) := -\frac{1}{2}\mathrm{Tr}\,(\Delta_x \hat{\varrho}) = \frac{1}{2}\mathrm{Tr}\,(|\nabla|\hat{\varrho}|\nabla|) \geq 0 \qquad \text{since } \hat{\varrho} \geq 0\,.$$

Table 2 Macroscopic quantities of a density matrix $\hat{\varrho}$

Observables: operator A	Expectation value $\mathrm{Tr}\,(A\hat{\varrho})$	Expectation value $\int_{\mathbb{R}^N} A_x \varrho\big\vert_{x=y} \mathrm{d}x$
x ... position	$\mathrm{Tr}\,(x\ \hat{\varrho})$	$\int x\varrho(x,x)\,\mathrm{d}x$
$-\mathrm{i}\nabla_x$ ... momentum	$-\mathrm{i}\mathrm{Tr}\,(\nabla_x\hat{\varrho})$	$-\mathrm{i}\int(\nabla_x\varrho)(x,x)\,\mathrm{d}x$
$-\frac{1}{2}\Delta_x$ ... kinetic energy	$-\frac{1}{2}\mathrm{Tr}\,(\Delta_x\hat{\varrho})$	$\frac{1}{2}\int(\nabla_x\cdot\nabla_y\varrho)(x,x)\,\mathrm{d}x$
$V(x)$ ... potential energy	$\mathrm{Tr}\,(V(x)\ \hat{\varrho})\geq 0$ if $V\geq 0$	$\int V(x)\varrho(x,x)\,\mathrm{d}x$

Here, $|\nabla|=\sqrt{-\Delta}$ is a pseudo-differential operator (ΨDO) with the symbol $|\xi|$, i.e. $(|\nabla|f)(x)=\mathcal{F}^{-1}(|\xi|(\mathcal{F}f)(\xi))\ \ \forall f\in H^1(\mathbb{R}^n)$.

More generally, we now illustrate how to compute from a density matrix its macroscopic observable that corresponds to a self-adjoint operator A (cf. also Sect. 1.1 and Table 1). If a quantum system is in state $\hat{\varrho}$ (or analogously described by $\varrho(x,y)$), the expectation value of the observable A is given by $\mathrm{Tr}\,(A\hat{\varrho})$ or $\int_{\mathbb{R}^N} A_x\varrho\Big|_{x=y}\mathrm{d}x$, resp. In the latter case A_x denotes the realization of the operator A, acting on the x-variable. The most important examples are summarized in Table 2.

We now collect some analytic tools needed for the self-consistent problem. For mixed quantum states, $\hat{\varrho}\in\tilde{\mathcal{J}}_1$ is the analogue of $\psi\in L^2$ in the pure state case. For the related Schrödinger–Poisson equation, a simple analysis was possible in the *energy space* $\psi\in H^1$ (cf. Sect. 3.1). We now give a corresponding density matrix framework that again allows to control the kinetic energy (as needed for the self-consistent potential).

With the ΨDO $\sqrt{1-\Delta}$ we define the *energy space*

$$\mathcal{E}:=\left\{\hat{\varrho}\in\tilde{\mathcal{J}}_1\ \middle|\ \sqrt{1-\Delta}\,\hat{\varrho}\,\sqrt{1-\Delta}\in\mathcal{J}_1\right\},$$

which is a Banach space with the norm

$$\|\hat{\varrho}\|_{\mathcal{E}}:=\|\sqrt{1-\Delta}\hat{\varrho}\sqrt{1-\Delta}\|_1\,.$$

For $\hat{\varrho}\geq 0$ it holds

$$\|\hat{\varrho}\|_{\mathcal{E}}=\mathrm{Tr}\,((1-\Delta)\hat{\varrho})=\mathrm{Tr}\,\hat{\varrho}+2E_{kin}(\hat{\varrho})\,.$$

In order to estimate the particle density n, and hence the self-consistent potential V in terms of $\hat{\varrho}$ (analogously to (18)) we shall need the following *Lieb–Thirring-type inequality* [LT76, LP93, Arn96]. This is a collective Sobolev or Gagliardo–Nierenberg inequality.

Lemma 4.1 ([Arn96]). *Let* $1 \le p \le \frac{N}{N-2}$ *(or* $1 \le p \le \infty$ *if* $N = 1$; $1 \le p < \infty$ *if* $N = 2$*) and* $\theta := \frac{N-p(N-2)}{2p} \in [0,1]$. *Then*

$$\|n[\hat{\varrho}]\|_{L^p(\mathbb{R}^N)} \le C_p \|\!|\hat{\varrho}|\!\|_1^\theta \, E_{kin}(|\hat{\varrho}|)^{1-\theta}, \qquad \forall \hat{\varrho} \in \mathcal{E}$$

Proof (for $N \ge 3$*).*
Consider $p = 1$, $\theta = 1$:

$$\|n\|_{L^1} \le \|\!|\hat{\varrho}|\!\|_1 \quad \text{follows from (23)}\,.$$

Consider $p = p_* := \frac{N}{N-2}$, $\theta = 0$: Then,

$$\|n\|_{L^{p_*}} \le \sum_j |\lambda_j| \, \|\psi_j\|_{L^{2p_*}}^2 \le C \sum_j |\lambda_j| \, \|\nabla\psi_j\|_{L^2}^2 = 2CE_{kin}(|\hat{\varrho}|)$$

follows by the Sobolev inequality. And the general case follows by interpolation. □

Remark 4.2. *A similar result with* $\|\!|\hat{\varrho}|\!\|_q^\theta$, $q > 1$ *on r.h.s. was obtained in [LP93]. Its proof is much harder.*

4.3 Time Evolution of Closed/Hamiltonian Systems

Assume that the time evolution of a wave function is determined by the *Hamiltonian* H, e.g. $H(t) = -\frac{1}{2}\Delta + V(t)$. The Schrödinger equation for a general pure state then reads

$$\mathrm{i}\psi_t = H\psi, \quad t \in \mathbb{R}\,. \tag{25}$$

Next we consider the eigenfunction decomposition for ϱ:

$$\varrho(x,y,t) = \sum_j \lambda_j \psi_j(x,t)\bar{\psi}_j(y,t)\,. \tag{26}$$

Using (25) in (26) yields the evolution equation for the density matrix. If $\hat{\varrho} \in \tilde{\mathcal{J}}_2$ or equivalently $\varrho(.,.,t) \in L^2(\mathbb{R}^{2N})$, this evolution can be written as a PDE for the kernel $\varrho(t)$ (cf. Remark 4.1):

$$\mathrm{i}\varrho_t = (H_x - H_y)\varrho, \quad t \in \mathbb{R}\,. \tag{27}$$

Here, H_x and H_y denote copies of the Hamiltonian H acting, resp., on the x- and y-variable. This is called the *quantum Liouville* or *von Neumann equation* (in coordinate representation).

However, if $\hat{\varrho} \in \tilde{\mathcal{J}}_1$, its evolution cannot be written as a PDE (cf. Remark 4.1). Instead, one has to write it as an abstract evolution problem (Banach space-ODE) for $\hat{\varrho}(t)$:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\varrho} = [H, \hat{\varrho}] := H\hat{\varrho} - \hat{\varrho}H, \quad t \in \mathbb{R}\,. \tag{28}$$

Also this variant of (27) is called *quantum Liouville* or *von Neumann equation.*

In order to solve it, we first consider the free Hamiltonian $H_0 := -\frac{1}{2}\Delta$. According to (28), the corresponding infinitesimal generator of the C_0-group $G_0(t),\ t \in \mathbb{R}$, for the $\hat{\varrho}$-evolution formally reads $h_0 = -\mathrm{i}[H_0, \hat{\varrho}]$. $G_0(t)$ has the following explicit representation:

$$G_0(t)\hat{\varrho} = \mathrm{e}^{-\mathrm{i}H_0 t}\hat{\varrho}\mathrm{e}^{\mathrm{i}H_0 t}\,, \quad t \in \mathbb{R}\,, \tag{29}$$

with the kernel

$$\sum_j \lambda_j (\mathrm{e}^{-\mathrm{i}H_0 t}\psi_j)(x)\,(\mathrm{e}^{\mathrm{i}H_0 t}\bar{\psi}_j)(y)\,.$$

One can see that the density matrix $\hat{\varrho}(t)$ solving (28) has eigenvalues that are constant in time. The corresponding eigenvectors obey the Schrödinger equation (25) and stay orthonormal during the evolution (which implies that they can only "rotate" in $L^2(\mathbb{R}^N)$).

The following lemma gives additional properties of the evolution group $G_0(t)$ and its generator h_0:

Lemma 4.2 ([DL88a]).

(a) $G_0(t)$ is a C_0-group of isometries on $\mathcal{J}_1$ It preserves self-adjointness and positivity.

(b) Its generator is characterized by

$$\begin{aligned}\mathcal{D}(h_0) \;&= \{\hat{\varrho} \in \mathcal{J}_1 \,\big|\, \hat{\varrho}\mathcal{D}(H_0) \subset \mathcal{D}(H_0), (H_0\hat{\varrho} - \hat{\varrho}H_0) \text{ is an operator with}\\ &\qquad \text{domain } H^2(\mathbb{R}^N) \text{ and it can be extended to } L^2(\mathbb{R}^N),\\ &\qquad \text{such that } \overline{H_0\hat{\varrho} - \hat{\varrho}H_0} \in \mathcal{J}_1\},\end{aligned}$$

$$h_0(\hat{\varrho}) \;:= -\mathrm{i}(\overline{H_0\hat{\varrho} - \hat{\varrho}H_0})\,.$$

Proof (of part (a)). The strong $\mathcal{J}_1$-continuity of $G_0(t)$ at $t = 0$ follows from the following two ingredients:

$$\|\!|G_0(t)\hat{\varrho}|\!\|_1 = \|\!|\hat{\varrho}|\!\|_1 \qquad \text{since } \lambda_j = \text{const. in } t \quad \text{(convergence of the } \mathcal{J}_1\text{−norm)},$$

$$\langle f, (G_0(t)\hat{\varrho})\, g\rangle = \langle \underbrace{\mathrm{e}^{\mathrm{i}H_0 t} f}_{\in C(\mathbb{R};L^2)}\,,\ \underbrace{\hat{\varrho}}_{\in\mathcal{B}(L^2)}(\mathrm{e}^{\mathrm{i}H_0 t} g)\rangle \xrightarrow{t\to 0} \langle f, \hat{\varrho}g\rangle \qquad \forall f,\, g \in L^2$$

(weak operator convergence).

These two properties imply the desired $\mathcal{J}_1$-convergence. This is a corollary to Grümm's Theorem (cf. [Sim79]).

The preservation of self-adjointness and positivity follows directly from (29). □

The above result for the evolution in $\mathcal{J}_1$ can easily be modified to an analogous result for the evolution in the energy space $\mathcal{E}$:

Corollary 4.1. *h_0 generates a C_0-group of isometries on $\mathcal{E}$.*

Proof. The operators $\sqrt{1-\Delta}$ and $\mathrm{e}^{-\mathrm{i}H_0t}$ commute. Hence:

$$\sqrt{1-\Delta}\,(G_0(t)\hat{\varrho})\,\sqrt{1-\Delta} = \mathrm{e}^{-\mathrm{i}H_0t}\,(\underbrace{\sqrt{1-\Delta}\hat{\varrho}\sqrt{1-\Delta}}_{\in\mathcal{J}_1})\,\mathrm{e}^{\mathrm{i}H_0t} \in C(\mathbb{R};\mathcal{J}_1)\,.$$

□

4.4 Von Neumann–Poisson Equation in $\mathbb{R}^3$

Here, we present the density matrix analogue of the H^1-analysis for a Schrödinger–Poisson system (SPS) (cf. Sect. 3.3). The von Neumann–Poisson equation for $\hat{\varrho}(t)$ discussed here is almost equivalent to the SPS-analysis in H^1: Via the SPS-analysis one constructs a corresponding solution $\hat{\varrho} \in C(\mathbb{R};\mathcal{E})$, hence the existence of a solution is guaranteed. However, its uniqueness in $\mathcal{J}_1$ or $\mathcal{E}$ would stay open.

Since the SPS-analysis is technically much simpler than the density matrix analysis, a $\mathcal{J}_1$-analysis would hence (almost) not be worth the effort for closed, i.e. Hamiltonian systems. However, the time evolution of open quantum systems (cf. Sect. 6) cannot be rewritten as a SPS. For such models, the $\hat{\varrho}$-analysis seems therefore unavoidable.

We start with the analysis of the *repulsive von Neumann–Poisson equation*:

$$\begin{cases} i\frac{d}{dt}\hat{\varrho}(t) = \overline{[-\frac{1}{2}\Delta + V(t), \hat{\varrho}(t)]}, \quad t \in \mathbb{R} \\ V(t) = \frac{1}{4\pi|x|} * n[\hat{\varrho}(t)] \\ \hat{\varrho}(0) = \hat{\sigma} \end{cases} \tag{30}$$

Theorem 4.3. *Let $\hat{\sigma} \in \mathcal{E}$. Then (30) has a unique solution $\hat{\varrho} \in C(\mathbb{R};\mathcal{E})$. It satisfies $\|\!|\hat{\varrho}(t)|\!\|_1 = \|\!|\hat{\sigma}|\!\|_1$.*

Proof. Morally, we follow the proof of Theorem 3.1. But since we are dealing with the evolution of operators instead of functions, we have to cope with many technical difficulties (Lieb–Thirring-type inequality instead of Sobolev inequality, e.g.):

1. $G_0(t)$ is a C_0-group of isometries on $\mathcal{J}_1$, $\tilde{\mathcal{J}}_1$, $\mathcal{E}$ (see Sect. 4.3).
2. $f(\hat{\varrho}) := -\mathrm{i}[V[\hat{\varrho}], \hat{\varrho}]$ is locally Lipschitz in $\mathcal{E}$ (but *not* in $\tilde{\mathcal{J}}_1$):
   - $\hat{\varrho} \in \mathcal{E} \;\Rightarrow\; V[\hat{\varrho}] \in L^\infty(\mathbb{R}^3)$ by (18) and the Lieb–Thirring-type inequality from Lemma 4.1.
   - We need to show that $\sqrt{1-\Delta}\,(V\hat{\varrho})\sqrt{1-\Delta} \in \mathcal{J}_1$:
     (a) First we decompose the ΨDO $\sqrt{1-\Delta}$ as follows:

$$\sqrt{1-\Delta} = 1 + \sum_j \underbrace{K_j}_{\in\mathcal{B}(L^2)} \partial_{x_j}\,.$$

This allows to use the product rule for $(V\hat{\varrho})$. Here, K_j is a ΨDO with the symbol

$$\mathrm{i}\frac{\xi_j}{|\xi|^2}\big(\sqrt{1+|\xi|^2}-1\big)$$

     (b) Next we need to show that $V\hat{\varrho}\sqrt{1-\Delta},\ \nabla(V\hat{\varrho}\sqrt{1-\Delta}) \in \mathcal{J}_1$. For the first term we use that

$$\sqrt{1-\Delta}\,\hat{\varrho}\sqrt{1-\Delta} \in \mathcal{J}_1 \overset{\hat{\varrho}\geq 0}{\Longrightarrow} \hat{\varrho}^{\frac{1}{2}}\sqrt{1-\Delta}\,,\ \ \hat{\varrho}^{\frac{1}{2}} \in \mathcal{J}_2\,.$$

For simplicity we assumed here first that $\hat{\varrho} \geq 0$ (but it can be generalized). Next, the "Hölder inequality" for the operator spaces $\mathcal{J}_p$ (cf. [RS75]) yields

$$\underbrace{V}_{\in\mathcal{B}}\,\underbrace{\hat{\varrho}^{\frac{1}{2}}}_{\in\mathcal{J}_2}\,\big(\underbrace{\hat{\varrho}^{\frac{1}{2}}\sqrt{1-\Delta}}_{\in\mathcal{J}_2}\big) \in \mathcal{J}_1\,.$$

3. Proposition 3.1 yields: The von Neumann–Poisson equation (30) has a *unique local solution* $\hat{\varrho} \in C([0,t_{max});\mathcal{E})$.
4. We have the a-priori estimates $\|\!|\hat{\varrho}(t)|\!\|_1 = \text{const}$ in t, $E_{kin}(\hat{\varrho}(t))$ is uniformly bounded (in t). Hence, the solution is global on $\mathbb{R}$.

□

Remark 4.4. *The quantum attractive case (with $V(t) = -\frac{1}{4\pi|x|} * n[\hat{\varrho}(t)]$) can be included with the following estimate (using the Lieb–Thirring-type inequality):*

$$-E_{pot}(\hat{\varrho}) := \|\nabla V\|_{L^2}^2 \leq C\|n\|_{\frac{6}{5}}^2 \leq C\|\!|\hat{\varrho}|\!\|_1^{\frac{3}{2}}\,E_{kin}(\hat{\varrho})^{\frac{1}{2}}$$

(cf. [Arn96]). A similar strategy also works for SP-analysis in Sect. 3.

5 Wigner Function Models

5.1 Wigner Functions

A Wigner function is obtained from the corresponding density matrix function by the *Wigner–Weyl transformation* (cf. [W32, SS87]):

$$\begin{aligned} w(x,v,t) &= (2\pi)^{-N/2}\mathcal{F}_{\eta\to v}\,\varrho\left(x+\frac{\hbar\eta}{2m}, x-\frac{\hbar\eta}{2m}, t\right) \\ &= (2\pi)^{-N}\sum_j \lambda_j \int_{\mathbb{R}^N} \psi_j(x+\frac{\hbar\eta}{2m},t)\bar{\psi}_j(x-\frac{\hbar\eta}{2m},t)e^{-iv\cdot\eta}\,\mathrm{d}\eta\,. \end{aligned}$$

Since $\varrho(x,y) = \overline{\varrho(y,x)}$, we have $w(x,v)\in\mathbb{R}$. Moreover,

$$w\in L^2(\mathbb{R}^{2N}) \Leftrightarrow \varrho\in L^2(\mathbb{R}^{2N}) \Leftrightarrow \hat{\varrho}\in\mathcal{J}_2(L^2(\mathbb{R}^N))\,.$$

We call w a *physical Wigner function*, if it corresponds to a density matrix $0\le\hat{\varrho}\in\tilde{\mathcal{J}}_1$.

Following [SS87] we now also give the direct transformation from the density matrix operator $\hat{\varrho}$ to the Wigner function w: With the *Weyl operators*

$$W(\xi,\eta) := e^{-i(\xi\cdot x - i\frac{\hbar}{m}\eta\cdot\nabla_x)}, \quad \text{for each } \xi,\eta\in\mathbb{R}^N$$

we have

$$w(x,v,t) = (2\pi)^{-2N}\iint_{\mathbb{R}^{2N}} \mathrm{Tr}\left(\hat{\varrho}(t)W(\xi,\eta)\right)e^{i(\xi\cdot x+\eta\cdot v)}\,\mathrm{d}\xi\mathrm{d}\eta\,.$$

Since the operators $\xi\cdot x - i\frac{\hbar}{m}\eta\cdot\nabla_x$ are essentially self-adjoint on $C_0^\infty(\mathbb{R}^N)$ $\forall\,\xi,\eta\in\mathbb{R}^N$ (cf. Lemma 5.1, Example 5.1, below), $W(\xi,\eta)$ is a unitary operator on $L^2(\mathbb{R}^N)$ by Stone's Theorem (cf. [Paz83]). Hence, $\mathrm{Tr}\left(\hat{\varrho}(t)W(\xi,\eta)\right)$ is well-defined for $\hat{\varrho}\in\mathcal{J}_1$ and each $\xi,\eta\in\mathbb{R}^N$.

The time evolution of w follows from the von Neumann equation: The *Wigner equation* reads

$$w_t + v\cdot\nabla_x w - e\,\Theta[V]w = 0, \quad x,v\in\mathbb{R}^N, t\in\mathbb{R}\,, \tag{31}$$

with the pseudo-differential operator (ΨDO)

$$\begin{aligned} &\Theta[V]w(x,v) \\ &= \frac{\mathrm{i}}{\hbar}(2\pi)^{-N}\iint_{\mathbb{R}^{2N}}\left[V(x+\frac{\hbar\eta}{2m}) - V(x-\frac{\hbar\eta}{2m})\right]w(x,\tilde{v})\mathrm{e}^{\mathrm{i}(v-\tilde{v})\cdot\eta}\,\mathrm{d}\tilde{v}\mathrm{d}\eta\,. \end{aligned}$$

In the *classical limit*, $\Theta[V]$ converges formally to its classical counterpart (see [LP93] for rigorous results). For a fixed function $w = w(x,v)$ and a fixed potential $V = V(x)$, we have:

$$\Theta[V]w \xrightarrow{\hbar\to 0} \frac{1}{m}\nabla_x V\cdot\nabla_v w\,.$$

For a quadratic potential V, the operator $\Theta[V]$ takes exactly the form of its classical counterpart:

$$\Theta[V]w = \frac{1}{m}\nabla_x V\cdot\nabla_v w\,. \tag{32}$$

In this special case the Wigner equation (formally) looks like the *classical Liouville equation*

$$f_t + v\cdot\nabla_x f - \frac{e}{m}\nabla_x V\cdot\nabla_v f = 0,\quad x,v\in\mathbb{R}^N\,. \tag{33}$$

Note that the Liouville equation and also the nonlinear Liouville–Poisson equation (also called *Vlasov–Poisson* equation) preserve all L^p-norms in time, i.e.

$$\|f(.,.,t)\|_{L^p(\mathbb{R}^{2N})} = \text{const. in } t\quad \forall 1\le p\le\infty,\ t\in\mathbb{R}\,.$$

This is implied by the fact that the solution of (33) is constant along its characteristics. In contrast, the Wigner equation (in general) only preserves the $L^2(\mathbb{R}^{2N})$-norm, since $v\cdot\nabla_x - e\,\Theta[V]$ is skew-adjoint.

If $V\in L^\infty(\mathbb{R}^N)$, then $\|\Theta[V]\|_{\mathcal{B}(L^2)}\le\frac{2}{\hbar}\|V\|_{L^\infty}$. Hence, in this case there exists a C_0-evolution group of isometries for the Wigner equation on $L^2(\mathbb{R}^{2N})$. This follows from Stone's theorem. Moreover, $\Theta[V]$ is a bounded perturbation of $v\cdot\nabla_x$.

From now on we set the parameters $e=m=\hbar=1$ and we recall the definition of the *macroscopic quantities* for a Wigner function w:

- Typical normalization of total mass: $\iint_{\mathbb{R}^{2N}} w\,\mathrm{d}x\mathrm{d}v = 1$
- Particle density: $n(x,t) := \int_{\mathbb{R}^N} w(x,v,t)\,\mathrm{d}v$ (≥ 0 for a physical Wigner function)
- Current density: $j(x,t) := \int_{\mathbb{R}^N} vw(x,v,t)\,\mathrm{d}v$
- Kinetic energy density: $e_{kin}(x,t) := \int_{\mathbb{R}^N}\frac{|v|^2}{2}w(x,v,t)\,\mathrm{d}v$ (≥ 0 for a physical Wigner function)

Note that these definitions are *purely formal* since a Wigner function satisfies $w(.,.,t)\in L^2(\mathbb{R}^{2N})$ but typically $w\notin L^1(\mathbb{R}^{2N})$. Hence, the "definition" $n :=$ "$\int w\,\mathrm{d}v$" is *meaningless*!

This is a key problem for analyzing the self-consistent Wigner–Poisson equation, i.e. (31) with the Coulomb potential obtained from $-\Delta V = n = \int w\,\mathrm{d}v$. In other words, the quadratically nonlinear term $\Theta[V[w]]w$ is *not defined pointwise in* t on the state space of the Wigner function ($w(t)\in L^2$, e.g.). This is the same problem like in the L^2-analysis of SP in Sect. 3.2. There are two simple solutions to this problem:

- Change the state space for w (even if it is not very physical): A weighted L^2-space with sufficient weight in the v-variable implies $w \in L^2_x(L^1_v)$ and hence $n \in L^2(\mathbb{R}^N_x)$. Possible options are:
  in 1D: $w \in L^2(\mathbb{R}^2; (1+v^2)\,\mathrm{d}x\,\mathrm{d}v)$, cf. [ACD02]
  in 3D: $w \in L^2(\mathbb{R}^6; (1+|v|^4)\,\mathrm{d}x\,\mathrm{d}v)$, cf. [ADM07]

- For Hamiltonian or closed systems (i.e. without collision operators in the Wigner equation) the Wigner–Poisson equation is (almost) equivalent to the SPS (Sect. 3.3). This allows for a much simpler analysis (cf. Theorem 3.3a, and [BM91, AN91, ILZ94, MRS90]).

5.2 Linear Wigner–Fokker–Planck: Well-Posedness

We shall now consider an *open quantum system* that includes a collision operator on the r.h.s. of (31). Such a model is *not* any more equivalent to a system of Schrödinger equations. Any mathematical analysis must hence be done on the level of Wigner functions or density matrices. In this and the next section we shall illustrate both approaches.

In this subsection and in Sect. 5.3 we analyze the linear *Wigner–Fokker–Planck equation* (WFP) with an external potential of the form $\frac{\mu}{2}|x|^2 + V(x)$, $\mu \in \mathbb{R}$, $V \in L^\infty(\mathbb{R}^N)$. Because of (32), the quadratic potential yields the classical potential term. Hence, the WFP equation reads:

$$\begin{cases} w_t + v\cdot\nabla_x w - \mu x\cdot\nabla_v w - \Theta[V]w = Qw\,, \qquad x,\, v \in \mathbb{R}^N,\, t>0 \\ Qw = \underbrace{D_{pp}\Delta_v w}_{\text{class. diffusion}} + \underbrace{2\gamma\,\mathrm{div}_v(vw)}_{\text{friction}} + \underbrace{D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_v w)}_{\text{quantum diffusion}} \\ w(x,v,t=0) = w_0(x,v) \end{cases} \tag{34}$$

- This model is quantum mechanically "correct" if the following *Lindblad condition* holds:
$$D_{pp}\,D_{qq} - D_{pq}^2 \geq \frac{\gamma^2}{4}\,. \tag{35}$$
Exactly in this case, (34) can be rewritten as a Lindblad equation (see (50) below) for the corresponding density matrix operator [ALMS04, SS87]. As a consequence, the positivity of the particle density is preserved under the time evolution: $n(x,t) \geq 0$, $\forall x,\, t$. Note that the "classical Fokker–Planck-term", i.e. the so-called *Caldeira–Leggett model* [CL83], with $D_{qq} = D_{pq} = 0$ does *not* satisfy the Lindblad condition (35). Nevertheless it is frequently used in applications, yielding reasonable results.
- The collision operator Qw models *diffusive effects* (e.g. the electron–phonon-interaction). Hence, (34) has applications for the electron transport in quantum semiconductors and for quantum Brownian motion.

- A derivation of (34) from the coupling of electrons to a bath of harmonic oscillators was given in [CEFM00].

Next we give an existence result for the linear WFP equation (34). The following theorem crucially depends on the *Lumer–Phillips Theorem* (cf. [Paz83]):

Proposition 5.1. *Let the operator A be densely defined and closed on the Banach space X. Let A and A^* be dissipative. Then, A generates a C_0-semigroup of contractions on X.*

We rewrite (34) as an evolution problem on $L^2(\mathbb{R}^{2N})$:

$$\begin{cases} w_t = Aw + \Theta[V]w, & t > 0\,, \\ w(0) = w_0 \in L^2(\mathbb{R}^{2N})\,, \end{cases} \tag{36}$$

with the abbreviation

$$\begin{aligned} Aw &:= -v\cdot\nabla_x w + \mu x\cdot\nabla_v w + Qw \\ &= -v\cdot\nabla_x w + \mu x\cdot\nabla_v w + 2\gamma\,\mathrm{div}_v(vw) \\ &+ D_{pp}\Delta_v w + 2D_{pq}\,\mathrm{div}_v(\nabla_x w) + D_{qq}\Delta_x w\,. \end{aligned}$$

Theorem 5.1. *Let $V \in L^\infty(\mathbb{R}^N)$ or $V \in L^1_{loc}\big(\mathbb{R}^+; L^\infty(\mathbb{R}^N)\big)$. Then (36) has a unique mild solution $w \in C\big([0,\infty); L^2(\mathbb{R}^{2N})\big)$.*

Proof.

- We define the operator $\tilde{A} := A - N\gamma$ on the domain $\mathcal{D}\big(\tilde{A}\big) := C_0^\infty\left(\mathbb{R}^{2N}\right)$.
- Then, $\tilde{A}$ is dissipative on $\mathcal{D}\big(\tilde{A}\big)$ and $\tilde{A}^*$ is (formally) *dissipative* in $L^2(\mathbb{R}^{2N})$, i.e. $\langle\tilde{A}w, w\rangle_{L^2} \le 0 \qquad \forall w \in \mathcal{D}\big(\tilde{A}\big)$. The rigorous proof of dissipativity for $\tilde{A}^*$ will follow from Lemma 5.1 below.

- From the Lumer–Phillips Theorem then follows: $\bar{\tilde{A}}$ generates a C_0-semigroup:
$$\left\|\mathrm{e}^{t\bar{\tilde{A}}}w\right\|_{L^2} \le \mathrm{e}^{N\gamma t}\,\|w\|_{L^2}\,, \quad t \ge 0\,. \tag{37}$$
- The final result follows, since $\Theta[V]$ is a bounded perturbation on $L^2(\mathbb{R}^{2N})$ (see Proposition 2.4 or 3.1, resp.).

□

Now we still have to prove the dissipativity of $\tilde{A}^*$ on $\mathcal{D}(\tilde{A}^*)$. Just like for $\tilde{A}$, one immediately finds that $\tilde{A}^*|_{\mathcal{D}(\tilde{A})}$ is dissipative, with

$$\tilde{A}^* = v\cdot\nabla_x w - \mu x\cdot\nabla_v w - 2\gamma\, v\cdot\nabla_v w + D_{pp}\Delta_v w + 2D_{pq}\,\mathrm{div}_v(\nabla_x w) + D_{qq}\Delta_x w - N\gamma\,.$$

However, $\mathcal{D}(\tilde{A}^*)$ is not known explicitly. To verify that $\tilde{A}^*$ is the closure of $\tilde{A}^*|_{\mathcal{D}(\tilde{A})}$ we shall use the following lemma, since $\tilde{A}^*$ is a quadratic polynomial in x, v, ∇_x, ∇_v:

Lemma 5.1 ([ACD02], [AS04]). *Let the operator $P = p_2(x, -i\nabla)$ be a quadratic polynomial in x, $-i\nabla$. Define the* minimum realization *of P on*

$$\mathcal{D}(P_{\min}) := C_0^\infty\left(\mathbb{R}^N\right) \subseteq L^2\left(\mathbb{R}^N\right) .$$

Then, $\overline{P_{\min}} = P_{\max}$, the maximum extension *of P, i.e.*

$$\mathcal{D}(P_{\max}) = \left\{f \in L^2 | Pf \in L^2\right\} .$$

Proof. For $f \in \mathcal{D}(P_{\max})$ we need to show, that it can be approximated in the graph norm $\|.\|_P$ by a sequence $\{f_n\} \subset C_0^\infty\left(\mathbb{R}^N\right)$. This is accomplished by the following (standard) approximation sequence (but the proof is lengthy):

$$f_n(x) := \underbrace{\chi_n(x)}_{C_0^\infty\text{-cutoff}} \cdot (f * \underbrace{\varphi_n}_{C_0^\infty\text{-mollifier}})(x) \overset{n\to\infty}{\longrightarrow} f \quad \text{in } \|.\|_P .$$

□

The following examples illustrate applications and limitations of this lemma:

Example 5.1. We consider several Schrödinger operators. Their essential self-adjointness on $C_0^\infty(\mathbb{R}^N)$ is crucial for the existence of a corresponding evolution group (cf. [RS75]).

(a) $P = -\Delta - |x|^2$, $\mathcal{D}(P) = C_0^\infty(\mathbb{R}^N)$ is essentially self-adjoint in $L^2(\mathbb{R}^N)$.
(b) $P = -\partial_x^2 + x^4$, $\mathcal{D}(P) = C_0^\infty(\mathbb{R})$ is also essentially self-adjoint in $L^2(\mathbb{R})$ [RS75]. Hence, Lemma 5.1 can be extended to this case of a positive quartic potential.
(c) $P = -\partial_x^2 - x^4$, $\mathcal{D}(P) = C_0^\infty(\mathbb{R})$ is *not* essentially self-adjoint in $L^2(\mathbb{R})$ [RS75]. Hence, Lemma 5.1 cannot be extended to this negative quartic potential. Note, that for this potential (classical) particles would run off to $x = \infty$ in finite time. Hence, no reversible, mass conserving dynamics can exist.

So we conclude, that Lemma 5.1 cannot be extended to all operators of the form $P = p_4(x, -\mathrm{i}\nabla)$ (i.e. quartic polynomials) – neither to all cubic polynomials, by the way.

5.3 Linear Wigner–Fokker–Planck: Large Time Behavior

First we consider the case of a quadratic external confinement potential $V(x) = \frac{\mu}{2}|x|^2$, $\mu \geq 0$. Because of (32), the linear *Wigner–Fokker–Planck equation* (WFP) then takes the form of a classical kinetic equation:

$$\begin{cases} w_t + v \cdot \nabla_x w - \mu x \cdot \nabla_v w = Qw\,, \qquad x,\, v \in \mathbb{R}^N,\, t > 0 \\ Qw := D_{pp}\Delta_v w + 2\gamma\,\mathrm{div}_v(vw) + D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_v w) \\ w(x,v,t=0) = w_0(x,v) w(x,v,t=0) = w_0(x,v) \in L^2(\mathbb{R}^{2N}) \end{cases} \tag{38}$$

Theorem 5.2 ([SCDM04]).

(a) (38) *has a Green's function* $G(x,v,x_0,v_0,t) \geq 0$ *(it is a non-isotropic Gaussian).*

(b) $\exists!$ *mild (and actually classical) solution of* (38)*:*

$$w(x,v,t) = \iint G(x,v,x_0,v_0,t) w_0(x_0,v_0)\,\mathrm{d}x_0\,\mathrm{d}v_0 \in C([0,\infty); L^2(\mathbb{R}^{2N}))\,. \tag{39}$$

When transforming (x,v) *to the characteristic coordinates of the Liouville equation* $w_t + v \cdot \nabla_x w - \mu x \cdot \nabla_v w = 0$*, the integral in* (39) *becomes a convolution in* x_0*,* v_0*.*

(c) $w_0(x,v) \geq 0 \;\Rightarrow\; w(x,v,t) \geq 0 \quad \forall t \geq 0\,.$

The dissipativity introduced by the collision operator Q and the confinement of the potential V makes the system converge to the equilibrium. This steady state w_∞ is unique up to the normalization of mass:

Theorem 5.3 ([SCDM04]). *Let* $\gamma > 0$ *and* $\mu > 0$*. Then*

(a) The WFP equation (38) *has a unique steady state (up to normalization of mass):*

$$w_\infty(x,v) = \mathrm{e}^{-[\alpha|x|^2 + 2\beta x\cdot v + \gamma|v|^2]}\,.$$

It is a non-isotropic $2N$*-dimensional Gaussian.*

(b) $w(t) \overset{t\to\infty}{\longrightarrow} w_\infty(x,v)$ *in relative entropy (cf.* (52)*),* $L^1(\mathbb{R}^{2N})$*, and in* $L^2(\mathbb{R}^{2N})$ *with an exponential rate. Here,* w_∞ *is normalized as*

$$\iint w_\infty \mathrm{d}x\mathrm{d}v = \iint w_0 \mathrm{d}x\mathrm{d}v\,.$$

Proof (of (b)).
This is an application of the *entropy method* (cf. [AMTU01]) for uniformly parabolic drift-diffusion equations with a uniformly convex "potential". The method is applied separately for the positive and negative part of the Wigner function: $w^{\pm}(x,v,t)$. □

Remark 5.4. *In contrast to classical kinetic models,* w_∞ *does* not *separately annihilate the collision term* Qw *and the transport term* $v \cdot \nabla_x w - \mu x \cdot \nabla_v w$ *in* (38)*. This reflects the non-local flavor of quantum mechanics.*

Next we present a recent extension of Theorem 5.3 for (small) perturbations λV_0 of the harmonic oscillator potential (cf. [AGGS07]). We consider

the linear WFP equation (36) with the identity as diffusion matrix (just for notational simplicity):

$$\begin{cases} w_t = Aw + \lambda\Theta[V_0]w, & t > 0\,, \\ w(0) = w_0, \end{cases} \tag{40}$$

with the abbreviation

$$\begin{aligned} Aw &:= -v\cdot\nabla_x w + x\cdot\nabla_v w + Qw \\ &= -v\cdot\nabla_x w + x\cdot\nabla_v w + 2\,\mathrm{div}_v(vw) + \Delta_v w + \Delta_x w\,. \end{aligned}$$

Let $w_\infty(x,v) > 0$ denote the unperturbed steady state (i.e. for $\lambda = 0$) from Theorem 5.3. It is unique when imposing the normalization $\iint_{\mathbb{R}^{2N}} w_\infty \mathrm{d}x\mathrm{d}v = 1$. We introduce the weighted Hilbert space $\mathcal{H} := L^2(\mathbb{R}^{2N}, w_\infty^{-1}\,\mathrm{d}x\mathrm{d}v)$.

Then we have

Theorem 5.5 ([AGGS07]). *Let $V_0 \in C^\infty(\mathbb{R}^N)$, such that $\hat{V}_0$ decays sufficiently fast (see [AGGS07] for the details), and let $|\lambda| > 0$ be sufficiently small. Then*

(a) The WFP equation (40) has a unique steady state $\tilde{w}_\infty \in \mathcal{H}$, satisfying the normalization condition $\iint_{\mathbb{R}^{2N}} \tilde{w}_\infty\,\mathrm{d}x\mathrm{d}v = 1$.

(b) For any initial function $w_0 \in \mathcal{H}$ with $\iint_{\mathbb{R}^{2N}} w_0\,\mathrm{d}x\mathrm{d}v = 1$ we have exponential convergence towards the steady state:

$$\|w(t) - \tilde{w}_\infty\|_{\mathcal{H}} \le \mathrm{e}^{-\varepsilon t}\|w_0 - \tilde{w}_\infty\|_{\mathcal{H}}, \qquad t \ge 0,$$

with some $\varepsilon > 0$.

Proof.

(a) We rewrite the stationary version of (40) as the fixed point problem

$$Aw = -\lambda\Theta[V_0]w$$

in order to use Banach's fixed point theorem. Since A has a non-trivial kernel (in fact $Aw_\infty = 0$ by Theorem 5.3), we cannot invert A. Hence we define $\mathcal{H}^\perp := \{f \in \mathcal{H} : f \perp w_\infty\}$ and modify the fixed point problem to

$$Az = -\lambda\Theta[V_0](z + w_\infty) \tag{41}$$

for $z := w - w_\infty \in \mathcal{H}^\perp$. Now, $\lambda A^{-1}\Theta[V_0]$ is contractive on $\mathcal{H}^\perp$ and its unique fixed point z^* yields the unique normalized steady state $\tilde{w}_\infty = z^* + w_\infty \in \mathcal{H}$ of (40).

(b) Consider on $\mathcal{H}^\perp$ the evolution of $v(t) := w(t) - \tilde{w}_\infty$, with $w(t)$ satisfying (40). Then, $\|v(t)\|_{\mathcal{H}}^2$ is a Lyapunov functional with exponential decay: For computing $\frac{\mathrm{d}}{\mathrm{d}t}\|v(t)\|_{\mathcal{H}}^2$ we use that the operator A has a spectral gap of size $\sigma = 1 - 1/\sqrt{2}$ on $\mathcal{H}$. Hence, its symmetric part A^s satisfies on $\mathcal{H}^\perp$: $A^s \le -\sigma$. The idea is now that the perturbation potential $\lambda\Theta[V_0]$ can be compensated by this spectral gap. □

5.4 Wigner–Poisson–Fokker–Planck: Global Solutions in $\mathbb{R}^3$

The Wigner–Poisson–Fokker–Planck (WPFP) system reads:

$$\begin{cases} w_t + v\cdot\nabla_x w - \Theta[V]w = Qw, \quad x,\, v\in\mathbb{R}^3,\ t>0 \\ Qw = \underbrace{D_{pp}\Delta_v w}_{\text{class. diffusion}} + \underbrace{2\gamma\,\mathrm{div}_v(vw)}_{\text{friction}} + \underbrace{D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_v w)}_{\text{quantum diffusion}} \\ -\Delta V(x,t) = n(x,t) := \int w(x,v,t)\,\mathrm{d}v \\ w(x,v,t=0) = w_0(x,v) \end{cases} \tag{42}$$

This is an open quantum systems with mean-field potential. For proving the existence of a global-in-time solution to (42) we face *two analytical problems:*

1. For $w\in L^2(\mathbb{R}^6)$ the nonlinear potential term is not locally Lipschitz. This makes the construction of a local-in-time solution difficult. Actually, the particle density $n(x,t)$ is not defined pointwise in time.
2. We lack enough (physical) a-priori estimates to establish a global-in-t solution.

First we discuss the *difficulties with the a-priori estimates*: For WPFP, the only simple a-priori estimate is (cf. (37))

$$\|w(t)\|_2 \le \mathrm{e}^{3\gamma t}\|w_0\|_2,\ t\ge 0,$$

which follows from the skew-adjointness of $v\cdot\nabla_x - \Theta[V]$. But we have *no* other L^p-estimates.

The physical conservation laws (like mass conservation $\iint w(x,v,t)\,\mathrm{d}x\,\mathrm{d}v = const$, or an energy balance involving the total kinetic energy $E_{kin}(t) = \frac{1}{2}\int\int |v|^2 w(x,v,t)\,\mathrm{d}x\,\mathrm{d}v$, cf. [ALMS04]) are *not* usable here, since $w\in\mathbb{R}$ (unless $\hat{\varrho}(t)\ge 0$ is used, as in [CLN04]).

The main idea for tackling both of the above problems is to find a *new a-priori estimate for the electric field* $E = E(x,t)$ in the WPFP equation. This will be used both:

- For the construction of the local-in-time solution via a fixed point map
- To establish the global-in-time solution

Since the particle density $n[w] = \int w\,\mathrm{d}v$ cannot be rigorously defined *pointwise in t*, we shall somehow eliminate it from the WPFP system. Instead, we shall define the electric field $E = -\nabla V = \frac{1}{4\pi}\frac{x}{|x|^3} * \int w\,\mathrm{d}v$ a.e. in t using the dispersive regularization of the free transport equation $w_t + v\cdot\nabla_x w = 0$.

A-Priori Estimate for Electric Field in Wigner–Poisson

We proceed similarly to [Per96] for the Vlasov–Poisson (VP) system, or [Cas98] for the Vlasov–Poisson–Fokker–Planck system.

To keep the notation simple we first illustrate the strategy for the Wigner–Poisson system, which reads in Duhamel form:

$$w(x,v,t) = w_0(x-vt,v) - \int_0^t (\Theta[V]w)(x-vs,v,t-s)\,\mathrm{d}s\,. \tag{43}$$

Using the particle density $n = \int w\,\mathrm{d}v$ from (43) we split the field as $E(x,t) = -\nabla V(x,t) = \frac{1}{4\pi}\frac{x}{|x|^3} * n(x,t) = E_0 + E_1$:

$$\begin{aligned} E_0(x,t) &:= \frac{1}{4\pi}\frac{x}{|x|^3} *_x \int w_0(x-vt,v)\,\mathrm{d}v\,,\\ E_1(x,t) &:= -\frac{1}{4\pi}\frac{x}{|x|^3} *_x \int_0^t \int_{\mathbb{R}^3_v} (\Theta[V]w)(x-vs,v,t-s)\,\mathrm{d}v\,\mathrm{d}s\,. \end{aligned} \tag{44}$$

For VP (studied in [Per96]) the corresponding term has the form

$$\begin{aligned} E_1(x,t) &= -\frac{1}{4\pi}\frac{x}{|x|^3} *_x \int_0^t\!\!\int (\nabla_x V\cdot\nabla_v w)(x-vs,v,t-s)\,\mathrm{d}v\,\mathrm{d}s\\ &= -\frac{1}{4\pi}\frac{x}{|x|^3} *_x \mathrm{div}_x \int_0^t s\!\int (\nabla_x V\, w)(x-vs,v,t-s)\,\mathrm{d}v\,\mathrm{d}s\,. \end{aligned} \tag{45}$$

Here, the key issue is that the second factor of this last convolution is in divergence form, in order to pass that div_x to the first convolution factor later on. Obviously, this is not the case in (44). However, with a tricky reformulation, $\Theta[V]$ can indeed be written in divergence form:

$$\Theta[V]w = \mathcal{F}^{-1}_{\eta\to v}\left(\delta V(x,\eta)\hat{w}(x,\eta)\right) = \nabla_x V *_x \Phi(x,v) *_v \nabla_v w,$$

with some distribution $\Phi(x,v)$ and

$$\delta V(x,\eta) = V(x+\frac{\eta}{2}) - V(x-\frac{\eta}{2}) = \int_{-\frac12}^{\frac12} \eta\cdot\nabla_x V(x-r\eta)\,\mathrm{d}r\,.$$

We illustrate this computation for the (simpler) 1D case:

$$\delta V(x,\eta)\hat{w}(x,\eta) = \eta\nabla_x V *_x \underbrace{\left(\frac{1}{|\eta|}\chi_{[-|\eta|/2,|\eta|/2]}\right)(x)}_{=:\hat{\Phi}(x,\eta)}\ \hat{w}(x,\eta)\,.$$

Following the strategy from (45), we can rewrite the components $j = 1,2,3$ of the field E_1 as

$$(E_1)_j(x,t) = \frac{1}{4\pi}\sum_{k=1}^{3}\frac{3x_jx_k-\delta_{jk}|x|^2}{|x|^5} *_x \int_0^t\!\!\int (\partial_{x_k} V *_x \Phi *_v w)(x-vs, v, t-s)\,\mathrm{d}v\,\mathrm{d}s\,.$$

This yields the following a-priori estimate for the WP case on any time interval $(0,T)$ [ADM07]:

Lemma 5.2. *Let* $w_0 \in L^2(\mathbb{R}^6)$ *and* $\left\|\int w_0(x-vt,v)\,\mathrm{d}v\right\|_{L^q_x(\mathbb{R}^3)} \le t^{-\omega_q}$, $t \le T$. *Then, it holds for* $0 < t \le T$*:*

$$\begin{aligned}\|E_1(t)\|_{L^2(\mathbb{R}^3)} &\le C\int_0^t s\,\mathrm{d}s \left\|\int (\nabla V *_x \Phi *_v w)(x-vs,v,t-s)\,\mathrm{d}v\right\|_{L^2_x(\mathbb{R}^3)}\\ &\le C\int_0^t \frac{s\,\mathrm{d}s}{s^{3/2}}\,\|(E_0+E_1)(t-s)\|_{L^2(\mathbb{R}^3)}\,\|w_0\|_{L^2(\mathbb{R}^6)}\,.\end{aligned}$$

Hence,

$$\|E_0(t)\|_{L^2(\mathbb{R}^3)} + \|E(t)\|_{L^2(\mathbb{R}^3)} \le Ct^{-\frac{3}{2q}+\frac{5}{4}-\omega_q}\,.$$

This lemma only provides an L^2-estimate on $E(t)$ for the WP system. For the VP system, however, one obtains a whole interval of L^p-estimates. This is due to the conservation of all norms $\|f(t)\|_{L^p(\mathbb{R}^6)}$, $1 \le p \le \infty$ in the VP case, while WP only conserves the L^2-norm in time.

A-Priori Estimate for Electric Field in WPFP

The WPFP system reads

$$\begin{aligned} w_t &= Aw + \Theta[V]w\,,\\ -\Delta V(x,t) &= n(x,t) := \int w(x,v,t)\,\mathrm{d}v\,,\end{aligned}$$

with the abbreviation

$$Aw := -v\nabla_x w + 2\gamma\,\mathrm{div}_v(vw) + D_{pp}\Delta_v w + D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_v w)\,.$$

Using the Green's function $G(x,v,x_0,v_0,t)$ from Theorem 5.2, the WPFP solution can be written in Duhamel form:

$$\begin{aligned} w(x,v,t) = &\iint_{\mathbb{R}^6} G(x,x,x_0,v_0,t)w_0(x_0,v_0)\,\mathrm{d}x_0\,\mathrm{d}v_0\\ &- \int_0^t\!\!\iint_{\mathbb{R}^6} G(x,x,x_0,v_0,s)(\Theta[V]w)(x_0,v_0,t-s)\,\mathrm{d}x_0\,\mathrm{d}v_0\,\mathrm{d}s\,.\end{aligned}$$

Proceeding like for the WP case, we obtain an a-priori estimate on the field for the WPFP system [ADM07]:

Lemma 5.3. *Let* $w_0 \in L^2$ *and* $\left\| \int w_0(x-vt,v)\,\mathrm{d}v \right\|_{L^q_x} \leq t^{-\omega_q}$, $t \leq T$. *Then, it holds for* $0 < t \leq T$*:*

$$\|E_0(t)\|_p + \|E(t)\|_p \leq Ct^{\frac{3}{2p}-\frac{3}{2q}+\frac{1}{2}-\omega_q},\ 2 \leq p < 6\,.$$

For $p > 2$, this result is obtained by the parabolic regularization of $G(t)$. Hence, this result goes beyond the WP-result in Lemma 5.2. For the iterative construction of the local-in-time solution we shall need in fact: $E \in L^1((0,T), L^3(\mathbb{R}^3))$. Hence, our procedure works for WPFP but not (yet) for WP.

Next we illustrate that the assumptions on w_0 in Lemmas 5.2, 5.3 can be obtained quite naturally. With the

Notation:

$$L^1_x(L^q_v) := L^1(\mathbb{R}^3_x; L^q(\mathbb{R}^3_v)), \quad 1 \leq q \leq \infty$$

we use the *Strichartz estimate* for the free transport equation [CP96]:

$$\left\| \int w_0(x-vt,v)\,dv \right\|_{L^q_x(\mathbb{R}^3)} \leq C\,|t|^{-3(1-\frac{1}{q})}\,\|w_0\|_{L^1_x(L^q_v)}\,, \quad t \in \mathbb{R}\,. \tag{46}$$

Hence, $w_0 \in L^1_x(L^q_v)$ yields exactly the needed assumption. When choosing some $q \in \left[1, \frac{6}{5}\right)$, (46) and Lemma 5.3 imply $\|E(t)\|_3 \in L^1(0,T)$, as needed.

Once we have an a-priori estimate for the field E on any $(0,T]$, we can define the potential V using the Poisson equation $\mathrm{div}E = n$:

$$V = \frac{1}{4\pi|x|} * n = \frac{1}{4\pi|x|} * \mathrm{div}E = -\frac{1}{4\pi}\sum_j \frac{x_j}{|x|^3} * E_j\,, \tag{47}$$

and analogously for the "split quantities" V_0, V_1, n_0, n_1 (cf. (44) for the splitting of E). This implies the following a-priori estimate on the self-consistent potential V:

Lemma 5.4. *Let* $w_0 \in L^2$*and* $\left\| \int w_0(x-vt,v)\,\mathrm{d}v \right\|_{L^q_x} \leq t^{-\omega_q}$, $t \leq T$. *Then, it holds for* $0 < t \leq T$*:*

$$\|V(t)\|_p \leq Ct^{\frac{3}{2p}-\frac{3}{2q}+1-\omega_q}, \quad 6 \leq p \leq \infty\,,$$

and hence

$$\Theta[V(t)] \in \mathcal{B}(L^2(\mathbb{R}^6)), \quad t > 0\,.$$

Definition of the Nonlinear Term $\Theta[V[w]]w$

The *standard definition* of the macroscopic quantities: density, self-consistent potential, and self-consistent field are made pointwise in time:

$$n(x,t)=\int w(x,v,t)\,\mathrm{d}v, \quad V(x,t)=\frac{1}{4\pi|x|}\ *_x\ n(x,t), \quad E(x,t)=-\nabla_x V(x,t)\,.$$

However, this is unfeasible for $w \in L^2$.

Therefore, we shall use the following *alternative definition*, which is nonlocal in t, via an integral equation for E_1. This is based on the above derivation of the a-priori estimate for E_1, and it yields a nonlinear map $w \mapsto E_1[w]$. We present it here for the WP case (to keep the notation simple), but the WPFP case is analogous:

$$\begin{aligned} &E_1[w]_j(x,t) \qquad (48)\\ &=-\frac{1}{4\pi}\sum_{k=1}^{3}\frac{3x_jx_k-\delta_{jk}|x|^2}{|x|^5}\ *_x\int_0^t s\int (E[w]_k\ *_x\ \Phi\ *_v\ w)(x-vs,v,t-s)\,\mathrm{d}v\,\mathrm{d}s\,. \end{aligned}$$

Using (47) we then obtain (the inhomogeneous parts of) the potential and density:

$$V_1[w]=-\frac{1}{4\pi}\sum_j \frac{x_j}{|x|^3} * E_1[w]_j, \qquad n_1[w]=-\Delta V_1[w]\,. \qquad (49)$$

Note that the a-priori estimate on $E_1[w]$ only depends on w_0 and $\|w(t)\|_2$ (cf. Lemmas 5.2, 5.3). Hence, $E_1[w] \in L^1((0,T);L^2(\mathbb{R}^3))$ is well-defined from (48) for all *Wigner trajectories* $w \in C([0,T];L^2(\mathbb{R}^6))$. For this definition $w(t)$ need *not* be the self-consistent Wigner function solving WPFP.

While the two above definitions of $E=E_0+E_1$ will generally be different, they coincide for the self-consistent solution w.

Iterative Construction of the WPFP Solution

For any time interval $[0,T]$ we now construct the WPFP solution by an iteration map M, defined on the following ball in a Banach space:

$$B_R=\left\{\, w\in C([0,T];L^2(\mathbb{R}^6)) \;\middle|\; \|w(t)\|_{L^2}\le R\right\},$$

with $R := \mathrm{e}^{3\gamma T}\,\|w_0\|_2$ reflecting the exponential growth of the L^2-norm: $\|w(t)\|_2 \le \mathrm{e}^{3\gamma t}\,\|w_0\|_2$.

In the (nonlinear) map M we first associate to w a potential $V[w]$ by (48), (49). Then, $\tilde{w}$ is the solution of the linear WFP (by Theorem 5.1):

$$\begin{aligned} \tilde{w}_t &= A\tilde{w} + \Theta[V[w]]\tilde{w}, \quad t \in (0,T]\,, \\ \tilde{w}(t{=}0) &= w_0\,. \end{aligned}$$

Summarizing we have

$$w \longmapsto \underbrace{V[w] = V_0 + V_1[w]}_{\in L^1((0,T);L^\infty(\mathbb{R}^3))} \longmapsto Mw := \tilde{w}\,.$$

Lemma 5.5. *Let* $w_0 \in L^2$ *and* $\left\| \int w_0(x-vt,v)\,\mathrm{d}v \right\|_{L^q_x} \leq t^{-\omega_q}$, $t \leq T$. *Then,* M^n *is a contraction on* B_R *for* $n = n(T)$ *large enough.*

This lemma implies that the WPFP system has a unique global-in-time solution:

Theorem 5.6 ([ADM07a]). *Let* $w_0 \in L^2_{x,v} \cap L^1_x\,(L^q_v)$ *for some* $1 \leq q < \frac{6}{5}$. *Then, WPFP has a unique* mild *solution:*

$$w \in C([0,\infty); L^2(\mathbb{R}^6)) \cap C((0,\infty); C^\infty_B(\mathbb{R}^6))\,,$$

$$n, V, E \in C((0,\infty); C^\infty_B(\mathbb{R}^3))\,.$$

Proof. For the existence of the mild solution combine Lemma 5.5 and (46). The regularity of w, n, V, E follows a-posteriori by using the regularization of the WPFP–Green's function. □

For other analytical approaches for the WPFP system we refer to [ALMS04, CLN04].

6 Open Quantum Systems in Lindblad Form

In a closed quantum system only interactions *within* that system exist. For an *open quantum system*, however, there actually exist two coupled systems: Firstly, our (finite) quantum system of interest, labeled S. And secondly, there exists a large reservoir (or "environment"), labeled R. If these two systems only interact with each other (but with no other external system), the coupled system $S + R$ forms a closed quantum system.

The idea of an open quantum system is now to model only the evolution of the small quantum system S: One includes the *uni-directional interaction* of R onto S, but one disregards the influence of S onto R. This is a reasonable approximation, if R is much larger than S. Henceforth we shall assume that R is in thermodynamic equilibrium (a "heat bath") that does not undergo a time evolution while interacting with S. As an example motivated by the discussion of Sect. 1.2, S might model an ensemble of electrons in a semiconductor crystal, while R models a phonon bath. For a general introduction to open quantum systems we refer to [AF01, AJP06, Dav76].

For the description of an open quantum system and its dynamics we make the following postulates:

- The open system S at time t is described by a density matrix $\hat{\varrho}(t) \in \tilde{\mathcal{J}}_1(\mathcal{H})$ with some Hilbert space $\mathcal{H}$.
- The dynamics of S is Markovian (i.e. there are no memory effects) and it is described by a conservative quantum dynamical semigroup (QDS) on $\mathcal{J}_1(\mathcal{H})$ (see below).

Definition 6.1. Let $G(t)$, $t \geq 0$ be a C_0-semigroup on some Hilbert space $\mathcal{H}$. Its dual map $G(t)^*$ on $\mathcal{B}(\mathcal{H})$ is called *completely positive*, if the tensor product

$$G(t)^* \otimes I_n \quad \text{defined on } \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathcal{H}_n)$$

is positivity preserving $\forall n \in \mathbb{N}$ (i.e. it maps positive operators to positive operators). Here, $\mathcal{H}_n$ denotes any n-dimensional Hilbert space, and I_n the n-dimensional unit matrix.

Definition 6.2. Let $G(t)$, $t \geq 0$ be a C_0-semigroup on $\mathcal{J}_1(\mathcal{H})$, with some Hilbert space $\mathcal{H}$. $G(t)$ is called a *conservative quantum dynamical semigroup*, if

- $G(t)$ is trace preserving, i.e. $Tr\hat{\varrho}(t) = Tr\hat{\varrho}(0)$, $t \geq 0$.
- $G(t)^*$ is *completely positive*.

Remark 6.1. *Complete positivity is clearly stronger than the positivity preservation. Moreover it is invariant under forming tensor products. This is important, if one wants to recover the dynamics of the coupled system $S + R$ from the dynamics of the open quantum system S.*

6.1 Lindblad Form

Theorem 6.2 (Structure of QDS-generators, [Lin76]). *Let $\mathcal{L}$ be the* bounded *generator of a QDS on $\mathcal{J}_1(\mathcal{H})$. Then, $\mathcal{L}$ is in* Lindblad form*:*

$$\mathcal{L}(\hat{\varrho}) = -i[H, \hat{\varrho}] + \sum_k \left(L_k \hat{\varrho} L_k^* - \frac{1}{2} \left(L_k^* L_k \hat{\varrho} + \hat{\varrho} L_k^* L_k \right) \right) ,$$

with some Hamiltonian $H \in \mathcal{B}(\mathcal{H})$ and (maybe countably many) Lindblad operators $L_k \in \mathcal{B}(\mathcal{H})$.

Remark 6.3. *The boundedness of $\mathcal{L}$ is important for the proof of Theorem 6.2. The extension of this result to arbitrary unbounded generators $\mathcal{L}$ is unknown. Nevertheless, this Lindblad structure of a QDS-generator is a useful and generally accepted assumption – also for the unbounded case!*

The most general type of a Markovian master equation describing the evolution of an open quantum system is the following *von Neumann equation* (also called *Lindblad equation* or *master equation in Lindblad form*):

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\varrho} &= \mathcal{L}(\hat{\varrho}) \\ &= -\mathrm{i}[H,\hat{\varrho}] + \underbrace{\sum_k \left(L_k \hat{\varrho} L_k^* - \frac{1}{2}\left(L_k^* L_k \hat{\varrho} + \hat{\varrho} L_k^* L_k\right)\right)}_{=:A(\hat{\varrho})} . \end{aligned} \tag{50}$$

Here, the operators H, L_k may be unbounded. As we shall see, the evolution of the density matrix $\hat{\varrho}(t)$ is now in general *non-unitary*.

We recall that at each t fixed, $\hat{\varrho}(t)$ admits a spectral decomposition

$$\hat{\varrho}(t) = \sum_{j\in\mathbb{N}} \lambda_j(t) \left|\psi_j(t)\right\rangle \left\langle\psi_j(t)\right| ,$$

where $\psi_j(t)$ are its eigenvectors and $\lambda_j(t)$ the eigenvalues. Here, $|\psi_j\rangle\langle\psi_j|$ denotes the projection operator onto the j-th eigenspace of $\hat{\varrho}(t)$. In contrast to a closed quantum system (cf. Sect. 4.3), the eigenvalues $\lambda_j(t)$ are *not* constant in time in the open quantum system (50). Hence, (50) cannot be reformulated as a Schrödinger system (cp. to Sects. 3.3, 4.3).

Moreover the dynamics is not time reversible, since the generator $\mathcal{L}$ is dissipative:

Definition 6.3. The operator A is called *dissipative*

(a) On a Hilbert $\mathcal{H}$, if

$$\Re\langle Ax, x\rangle \leq 0 \qquad \forall x \in \mathcal{D}(A) \subset \mathcal{H} ;$$

(b) On the Banach space $\tilde{\mathcal{J}}_1(\mathcal{H})$, if

$$\Re\, Tr\left(A(\hat{\varrho})\mathrm{sgn}(\hat{\varrho})\|\hat{\varrho}\|_1\right) \leq 0 \qquad \forall \hat{\varrho} \in \mathcal{D}(A) \subset \tilde{\mathcal{J}}_1(\mathcal{H}) .$$

Here, $\mathrm{sgn}(\hat{\varrho})$ is defined by the functional calculus.

Lemma 6.1. *A solution $\hat{\varrho}(t)$ of (50) formally satisfies:*

(a) Trace preservation;
(b) Positivity preservation, i.e. $\hat{\varrho}(0) \geq 0 \Rightarrow \hat{\varrho}(t) \geq 0 \quad \forall t \geq 0$;
(c) The generator $\mathcal{L}$ is dissipative in $\tilde{\mathcal{J}}_1(\mathcal{H})$.

Proof (purely formal, since $\mathcal{L}$ might not generate an evolution semigroup).

(a) From (50) it follows $\frac{d}{dt}\mathrm{Tr}\,\hat{\varrho}(t) = 0$, from the cyclic property of the trace.

(b) Let $\hat{\varrho} \geq 0$, and decompose $\mathcal{L}$ as:

$$\mathcal{L}_1(\hat{\varrho}) := \sum_k L_k \hat{\varrho} L_k^* \geq 0\,,$$
$$\mathcal{L}_2(\hat{\varrho}) := -(\tilde{H}\hat{\varrho} + \hat{\varrho}\tilde{H}^*), \quad \tilde{H} := \mathrm{i}H + \frac{1}{2}\sum_k L_k^* L_k\,.$$

Then, $\hat{\varrho} \geq 0$ and $\frac{\mathrm{d}}{\mathrm{d}t}\hat{\varrho} = \mathcal{L}_1(\hat{\varrho}) \geq 0$ imply $\mathrm{e}^{t\mathcal{L}_1}\hat{\varrho} \geq 0,\ \forall t \geq 0$. Moreover, $\mathcal{L}_2$ generates the evolution semigroup

$$\mathrm{e}^{t\mathcal{L}_2}\hat{\varrho} = \mathrm{e}^{-t\tilde{H}}\hat{\varrho}\mathrm{e}^{-t\tilde{H}^*}\,,$$

which preserves positivity. Now we conclude the positivity preservation of $\mathrm{e}^{t\mathcal{L}}$ by Trotter's product formula:

$$\mathrm{e}^{t\mathcal{L}} = \lim_{n\to\infty}\left[\mathrm{e}^{\frac{t}{n}\mathcal{L}_1}\mathrm{e}^{\frac{t}{n}\mathcal{L}_2}\right]^n\,.$$

(c) In the proof we split the Hamiltonian part from the Lindblad part $A(\hat{\varrho})$:

$$\mathrm{Tr}\,([H,\hat{\varrho}]\,\mathrm{sgn}(\hat{\varrho})) = \mathrm{Tr}\,(H|\hat{\varrho}| - |\hat{\varrho}|H) = 0\,;$$

$$\begin{aligned}
&\Re\,\mathrm{Tr}\,\left(L_k\hat{\varrho}L_k^*\,\mathrm{sgn}(\hat{\varrho}) - L_k|\hat{\varrho}|L_k^*\right)\\
&= \mathrm{Tr}\,\left(L_k^*\mathrm{sgn}(\hat{\varrho})L_k\hat{\varrho} - L_k^*L_k|\hat{\varrho}|\right)\\
&= \sum_j \langle L_k\psi_j\,,\,(\mathrm{sgn}(\hat{\varrho})L_k\hat{\varrho} - L_k|\hat{\varrho}|)\,\psi_j\rangle\\
&= \sum_j \lambda_j \underbrace{\langle L_k\psi_j\,,\,\mathrm{sgn}(\hat{\varrho})L_k\,\psi_j\rangle}_{\leq \|L_k\psi_j\|_{L^2}^2} - \sum_j |\lambda_j|\,\|L_k\psi_j\|_{L^2}^2 \leq 0\,,
\end{aligned}$$

with $(\psi_j,\,\lambda_j)$ denoting the eigenpairs of $\hat{\varrho}$. □

Now we give several examples of Lindblad operators L_k and compute its corresponding Wigner collision operators Q (cf. the discussion in Sect. 1.2).

Example 6.1. $L_1 = x \qquad \Rightarrow Qw = \frac{1}{2}\Delta_v w\,.$

Example 6.2. $L_1 = \nabla_x \quad \Rightarrow Qw = \frac{1}{2}\Delta_x w\,.$

Example 6.3. For the quantum Fokker–Planck term (in the Wigner formalism):

$$Qw = 2\gamma\,\mathrm{div}_v(vw) + D_{pp}\Delta_v w + 2D_{pq}\,\mathrm{div}_x(\nabla_v w) + D_{qq}\Delta_x w\,,$$

there exist $2N$ Lindblad operators L_k, such that the (linear) WFP equation (38) can be rewritten as a von Neumann equation in Lindblad form [ALMS04]. All of these L_k are in the form

$$L_k = \alpha_k \cdot x + \beta_k \cdot \nabla_x \,; \quad k = 1, \ldots, 2N \,.$$

Note that, for a given Lindblad part $A(\hat{\varrho})$ in (50) (or for a given Wigner collision operator Q, as in this example), its "decomposition" into the Lindblad operators L_k are typically *never* uniquely defined.

Example 6.4. For the Wigner-relaxation term $Qw = \frac{w_{st}-w}{\tau}$ with a constant relaxation time τ, we assume the normalization $\iint_{\mathbb{R}^{2N}} w_{st}\,\mathrm{d}x\mathrm{d}v = 1$. The density matrix $\hat{\varrho}_{st}$ corresponding to w_{st} hence satisfies $\operatorname{Tr}\hat{\varrho}_{st} = 1$, and it has an eigenfunction expansion of the form

$$\hat{\varrho}_{st} = \sum_{j\in\mathbb{N}} \mu_j |\phi_j\rangle \langle\phi_j| \,.$$

Here, $|\phi_j\rangle\langle\phi_j|$ denote the projection operators onto the eigenfunctions ϕ_j of $\hat{\varrho}_{st}$. Since $\operatorname{Tr}\hat{\varrho}_{st} = 1$, we rewrite the relaxation term for the density matrix as:

$$\frac{\hat{\varrho}_{st} - \hat{\varrho}}{\tau} = \frac{\hat{\varrho}_{st}\operatorname{Tr}\hat{\varrho} - \hat{\varrho}\operatorname{Tr}\hat{\varrho}_{st}}{\tau} \,.$$

And now it is in homogeneous w.r.t. $\hat{\varrho}$. With the (countably many) Lindblad operators

$$L_{jk} = \sqrt{\frac{\mu_k}{\tau}}\,|\phi_k\rangle\langle\phi_j|, \quad j,k \in \mathbb{N}$$

this relaxation term can be represented in Lindblad form [Arn96a].

We now turn to some remarks on techniques applied to investigate the large-time behavior of quantum dynamical semigroups. Consider a system that admits an equilibrium state. An interesting issue then is, if the system would converge to that equilibrium as $t \to \infty$. An example of such a question was studied in [FR98] for a class of Lindblad equations. But it is yet unexplored if those results apply to the evolution problems discussed here and in Sect. 6.2. Anyway, we shall now briefly review the (relative) quantum entropy as a possible tool for a future analysis of the large-time behavior of (50).

Quantum Entropy (Von Neumann Entropy)

The *quantum entropy* of a density matrix $\hat{\varrho}$ is defined as

$$S(\hat{\varrho}) := \operatorname{Tr}(\hat{\varrho}\ln\hat{\varrho}) \,.$$

For $0 \le \hat{\varrho} \le 1$ it satisfies $-\infty \le S(\hat{\varrho}) \le 0$.

Proposition 6.1 ([BN88]). *Let the Lindblad operators in* (50) *satisfy* $\sum_k L_k L_k^* \le \sum_k L_k^* L_k$. *Then*

$$\frac{\mathrm{d}}{\mathrm{d}t} S(\hat{\varrho}(t)) \le 0 \,, \qquad t \ge 0 \,.$$

Proof.

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}S(\hat{\varrho}(t)) &= \mathrm{Tr}\ (\hat{\varrho}_t \ln \hat{\varrho}) \\
&= \mathrm{Tr}\Big(\sum_k \big[L_k \hat{\varrho} L_k^* - L_k^* L_k \hat{\varrho}\big] \ln \hat{\varrho}\Big) \\
&= \sum_{j,k} \langle \psi_j\,,\, L_k\ \hat{\varrho} L_k^* \psi_j\rangle \ln \lambda_j - \langle \psi_j\,,\, L_k^*\ L_k\,\psi_j\rangle \lambda_j \ln \lambda_j \\
&\qquad \text{(Insert here } \sum_l |\psi_l\rangle\langle\psi_l| = \mathbb{1},\ \text{ the identity operator;} \\
&\qquad \text{the sum is understood in the strong operator sense.)} \\
&= \sum_{j,k,l} \langle \psi_j\,,\, L_k\,\psi_l\rangle\langle\psi_l\,,\, L_k^*\,\psi_j\rangle \lambda_l \ln \lambda_j \\
&\quad -\langle \psi_l\,,\, L_k^*\,\psi_j\rangle\langle\psi_j\,,\, L_k\,\psi_l\rangle \lambda_l \ln \lambda_l \qquad (j,\, l \text{ interchanged}) \\
&\le \sum_{j,k,l} |\langle \psi_j\,,\, L_k\,\psi_l\rangle|^2\,(\lambda_j - \lambda_l) \qquad (\text{use } \ln\frac{\lambda_j}{\lambda_l} \le \frac{\lambda_j}{\lambda_l} - 1) \\
&= \mathrm{Tr}\Big(\sum_k \big[L_k L_k^* - L_k^* L_k\big]\hat{\varrho}\Big) \\
&\le 0\,,
\end{aligned}
$$

with $(\psi_j,\, \lambda_j)$ denoting the eigenpairs of $\hat{\varrho}$. □

Remark 6.4. *The above result is sharp in the following sense. Assume that the condition* $\sum_k L_k L_k^* \le \sum_k L_k^* L_k$ *does not hold. Then there exists an initial condition* $\hat{\varrho}_0$*, such that the corresponding trajectory* $\hat{\varrho}(t)$ *satisfies* $\frac{\mathrm{d}}{\mathrm{d}t}S(\hat{\varrho}(t=0)) > 0$.

Applying this result to the Lindblad formulation of the WFP equation yields: $\sum_k L_k^* L_k - L_k^* L_k = -2N\gamma$. Hence, Proposition 6.1 can be applied only in the frictionless case ($\gamma = 0$) [ALMS04].

Relative Quantum Entropy

The *relative quantum entropy* is defined as

$$
S(\hat{\varrho}|\hat{\sigma}) := \mathrm{Tr}\ (\hat{\varrho}(\ln \hat{\varrho} - \ln \hat{\sigma})) \qquad \text{for } \hat{\varrho},\, \hat{\sigma} \in \tilde{\mathcal{J}}_1\,; \quad \hat{\varrho},\, \hat{\sigma} \ge 0\,,
$$

and it satisfies:

Proposition 6.2 ([AF01]). *Let dim* $\mathcal{H} < \infty$*, then:*

(a)

$$
\begin{aligned}
&S(\hat{\varrho}|\hat{\sigma}) \ge 0\,, \\
&S(\hat{\varrho}|\hat{\sigma}) = 0 \qquad \textit{iff}\ \ \hat{\varrho} = \hat{\sigma}\,.
\end{aligned}
$$

(b) Let $G(t)$, $t \geq 0$ be a conservative QDS. Then:

$$S(G(t)\hat{\varrho}\,|\,G(t)\hat{\sigma}) \leq S(\hat{\varrho}|\hat{\sigma}), \quad t \geq 0\,.$$

(c)

$$\frac{1}{2}\|\!|\hat{\varrho} - \hat{\sigma}|\!\|_1^2 \leq S(\hat{\varrho}|\hat{\sigma})\,. \tag{51}$$

Remark 6.5. *(b) + (c) imply the $\mathcal{J}_1$-stability of a steady state. For further results on the quantum entropy (production) in finite dimensional systems cf. [Spo76, Spo78].*

As a comparison we briefly recall the notion of *classical relative entropy*, which is frequently used for analyzing the large-time behavior of linear and non-linear parabolic equations and of (classical) kinetic equations via the so-called *entropy method* (cf. [AMTU01, Arn02]). For two probability densities f, $g \in L^1\left(\mathbb{R}^N\right)$ the *relative entropy* is defined as

$$e(f|g) := \int_{\mathbb{R}^N} \frac{f}{g} \ln\left(\frac{f}{g}\right) \mathrm{d}g \geq 0. \tag{52}$$

It satisfies the *Csiszár–Kullback* inequality:

$$\frac{1}{2}\,\|f - g\|_{L^1}^2 \leq e(f|g),$$

which is formally equivalent to inequality (51).

6.2 Quantum Fokker–Planck Equation

In this subsection we reconsider the Wigner–Poisson–Fokker–Planck system in $\mathbb{R}^6$:

$$\begin{cases} w_t + v \cdot \nabla_x w - \Theta[V]w = Qw\,, \\ Qw = \underbrace{D_{pp}\Delta_v w}_{\text{class. diffusion}} + \underbrace{2\gamma\,\mathrm{div}_v(vw)}_{\text{friction}} + \underbrace{D_{qq}\Delta_x w + 2D_{pq}\,\mathrm{div}_x(\nabla_v w)}_{\text{quantum diffusion}} \\ -\Delta V(x,t) = n(x,t) := \int w(x,v,t)\,\mathrm{d}v\,, \\ w(x,v,t=0) = w_0(x,v)\,. \end{cases} \tag{53}$$

But now we shall analyze its well-posedness on the level of density matrices.

As already mentioned in Remark 4.1, the time evolution of a density matrix can either be consider in terms of a PDE for the density matrix function $\varrho(x,y)$ or as an abstract evolution problem (in the space of trace class operators) for the density matrix operator $\hat{\varrho}$:

We have $\hat{\varrho} \in \mathcal{J}_2(L^2(\mathbb{R}^N)) \Leftrightarrow \varrho(x,y) \in L^2(\mathbb{R}^{2N})$. Hence, we can write a PDE for the time evolution of the function $\varrho(x,y,t)$:

$$\begin{aligned}\varrho_t = &-\mathrm{i}(H_x - H_y)\varrho - \gamma(x-y)\cdot(\nabla_x - \nabla_y)\varrho \\ &+ \left[D_{qq}|\nabla_x + \nabla_y|^2 - D_{pp}|x-y|^2 + 2\mathrm{i}D_{pq}(x-y)\cdot(\nabla_x + \nabla_y)\right]\varrho\,,\end{aligned} \tag{54}$$

with the Hamiltonian $H_x = -\frac{1}{2}\Delta_x + V(x,t)$ (and analogously for H_y).

However, the L^2-setting is not enough since we also consider $\hat{\varrho} \in \mathcal{J}_1$. In this case, there exists no "nice" space to characterize the corresponding kernel $\varrho(x,y)$. And hence, we cannot use the PDE (54) for the time evolution of the function $\varrho(x,y)$. Instead we have to employ the following evolution equation of the time-dependent operator $\hat{\varrho}(t)$:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{\varrho} = &-\mathrm{i}[\tilde{H}, \hat{\varrho}] \\ &+ \underbrace{\sum_k L_k \hat{\varrho} L_k^* - \frac{1}{2}\left(L_k^* L_k \hat{\varrho} + \hat{\varrho} L_k^* L_k\right)}_{=:A(\hat{\varrho})}\,,\end{aligned} \tag{55}$$

with the "adjusted" Hamiltonian

$$\tilde{H} = -\frac{1}{2}\Delta_x + V(x,t) - \mathrm{i}\frac{\gamma}{2}\{x, \nabla\}\,,$$

and $2N$ Lindblad operators of the form

$$L_k = \alpha_k \cdot x + \beta_k \cdot \nabla_x, \quad k = 1, \ldots, 6 = 2N.$$

Equation (55) is equivalent to (53) with the appropriate L_k's (see [ALMS04] for details).

Since we shall eventually discuss here the self-consistent quantum Fokker–Planck–Poisson (QFPP) problem (54) coupled to the Poisson equation

$$-\Delta V(x,t) = n(x,t),$$

we need to use the operator framework, in order to properly define the particle density n and the potential V (cf. Remark 4.1).

Our subsequent analysis parallels the strategy of Theorem 3.1 (i.e. the H^1-analysis of SP in 3D), and we split it in three steps.

(a) Linear case:
As before, we first consider the linear QFP equation (54) with V given.

For a general Lindblad equation

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\hat{\varrho} = \mathcal{L}(\hat{\varrho}) := -\mathrm{i}[\tilde{H}, \hat{\varrho}] + A(\hat{\varrho}), \quad t \geq 0 \\ \hat{\varrho}(t{=}0) = \hat{\varrho}_0 \end{cases} \tag{56}$$

with the dissipative/Lindblad terms $A(\hat{\varrho})$ introduced in (55), Davies [Dav77] constructed a linear C_0-evolution semigroup on $\mathcal{J}_1$. However, without special assumptions on the Hamiltonian $\tilde{H}$ and the Lindblad terms $A(\hat{\varrho})$, this so-called "minimal solution" can exhibit the following problems, which are closely related to each other:

- The semigroup, and hence the solution to (56) may be *not* unique.
- The domain $\mathcal{D}(\mathcal{L})$ might be "too small".
- The semigroup may be *not* conservative, i.e. $\mathrm{Tr}\,(\hat{\varrho}(t)) < \mathrm{Tr}\ \hat{\varrho}_0$ is possible for some $t > 0$.

Indeed, there exist examples where these problems occur.
One possibility to check that they do not happen for a specific problem at hand, is to prove that $\mathcal{D}(\overline{\mathcal{L}})$ is "big enough". For our QFP equation (54) this can be accomplished with the following lemma. It is an extension of Lemma 5.1 to mappings on operator spaces.

Lemma 6.2 ([AS04]). *Let $\mathcal{L}$ be quadratic in x and ∇_x. Then $\overline{\mathcal{L}|_{\mathcal{D}_\infty}}$ is the "maximum extension" in $\mathcal{J}_1$, in the sense that*

$$\mathcal{D}\left(\overline{\mathcal{L}|_{\mathcal{D}_\infty}}\right) = \mathcal{D}(\mathcal{L}_{\max}) := \{\hat{\varrho} \in \mathcal{J}_1 \,\big|\, \mathcal{L}(\hat{\varrho}) \in \mathcal{J}_1\}\,.$$

Here, $\mathcal{D}_\infty$ is a dense subset of $\mathcal{J}_1$-operators with C_0^∞-kernels ϱ (for the precise definition cf. [AS04]). It plays the same role as the C_0^∞-functions in Lemma 5.1.

Proof. For $\hat{\varrho} \in \mathcal{D}(\mathcal{L}_{\max})$ we need to construct a sequence $\{\hat{\sigma}_n\}_{n\in\mathbb{N}} \subset \mathcal{D}_\infty$, such that

$$\hat{\sigma}_n \overset{n\to\infty}{\longrightarrow} \hat{\varrho} \quad \text{in the graph norm } \|.\|_{\mathcal{L}}\,.$$

Their kernels can be obtained by

$$\sigma_n(x,y) := \underbrace{\chi_n(x)}_{C_0^\infty\text{-cutoff}} \big[\, \varphi_n(x) *_x \varrho(x,y) *_y \underbrace{\varphi_n(y)}_{C_0^\infty\text{-mollifier}} \,\big] \chi_n(y)\,.$$

□

This yields the following result for the linear QPF equation (54) on $\tilde{\mathcal{J}}_1(L^2(\mathbb{R}^N))$:

Theorem 6.6. *For the QFP equation, the C_0-semigroup $\mathrm{e}^{\mathcal{L}t}$ constructed by Davies in [Dav77] is unique and trace preserving.*

As a next step we consider the linear QFP equation on the energy space $\mathcal{E}$, defined in Sect. 4.2. Indeed, $\mathrm{e}^{\mathcal{L}t}$ is a C_0-semigroup also in $\mathcal{E}$. Since Davies' semigroup construction only holds in $\mathcal{J}_1$, one needs to prove explicitly the strong continuity of $\mathrm{e}^{\mathcal{L}t}$ w.r.t. t in $\mathcal{E}$ (obtained by Grümm's Theorem, see [Sim79]).

(b) Nonlinear case – local solution:
Now we turn to the nonlinear QFPP equation in 3D. Like in Theorem 3.1 we prove that the nonlinear Hartree-term $[V[\hat{\varrho}], \hat{\varrho}]$ (in (55)) is a local Lipschitz map in $\mathcal{E}$ – but it is not in $\mathcal{J}_1$ (this was the reason for making the analysis in $\mathcal{E}$). To this end one uses the following two estimates on the particle density: (23) and

$$\|n[\hat{\varrho}]\|_{L^3(\mathbb{R}^3)} \leq C|\!|\!|\hat{\varrho}|\!|\!|_{\mathcal{E}}$$

from Lemma 4.1.
Proposition 3.1 then implies that the QFPP equation has a local-in-t solution $\hat{\varrho} \in C([0, t_{max}); \mathcal{E})$.

(c) Nonlinear case – global solution:
To show that the solution exists for all time, we use the following a-priori estimates on the total mass:

$$\operatorname{Tr} \hat{\varrho}(t) = \text{ const. in } t, \qquad \hat{\varrho}(t) \geq 0 \quad \text{(see Lemma 6.1)},$$

and on the total energy, defined as

$$E_{\text{tot}}(\hat{\varrho}) := E_{\text{kin}}(\hat{\varrho}) + \frac{1}{2} \|\nabla_x V[\hat{\varrho}]\|_{L^2}^2 \ .$$

The latter satisfies (cf. [ALMS04])

$$\frac{\mathrm{d}}{\mathrm{d}t} E_{\text{tot}} = 3\, D_{pp} \operatorname{Tr} \hat{\varrho}_0 - 4\gamma\, E_{\text{kin}}(t) - D_{qq}\ \|n(t)\|_{L^2}^2 \ .$$

Finally we obtain:

Theorem 6.7 ([AS04]). *Let $\hat{\varrho}_0 \in \mathcal{E}$ and $\hat{\varrho}_0 \geq 0$. Then, there exists a global-in-time, positive, trace preserving, finite energy solution $\hat{\varrho} \in C([0, \infty); \mathcal{E})$ of the QFPP system* (55).

Let us briefly compare this theorem to the Wigner function approach of Sect. 5.4. The advantage of the density matrix approach for the QFPP system is that we work in the physical energy space $\mathcal{E} := \{\hat{\varrho} \in \mathcal{J}_1 | E_{\text{kin}}(\hat{\varrho}) < \infty\}$. Moreover, we only use physically important and meaningful a-priori estimates (for the total mass, kinetic energy, total energy). Hence, these estimates are much easier to derive than the rather technical estimate on $\|E(t)\|_{L^2}$ in Sect. 5.4.

However, if we would want to generalize the result to bounded domain problems, the density matrix formalism would not be appropriate, and we would need to pass to the Wigner formalism (53).

We finally remark, that a result similar to Theorem 6.7 was obtained in [Arn96] for the relaxation-time Wigner–Poisson system and its density matrix analogue.

7 Wigner Boundary Value Problems

In Sect. 1.2 we presented a relaxation-time Wigner–Poisson model for a resonant tunneling diode. This was an IBVP on the phase space slab $(x, v) \in (0, L) \times \mathbb{R}$ with inflow boundary conditions (BCs). In this section we shall discuss the linear Wigner boundary value problem (BVP), first in the stationary case in one spatial dimension and then the large-time behavior of the transient problem.

7.1 1D Stationary Boundary Value Problem

Here we shall discuss the existence and uniqueness of a solution $w(x, v)$ to the BVP for the linear, stationary Wigner equation in 1D with prescribed inflow BCs f^+, f^-:

$$\left\{ \begin{array}{rcll} v w_x - \Theta[V]w &=& 0, & 0 < x < L, \quad v \in \mathbb{R}\,, \\ w(0, v) &=& f^+(v), & v > 0\,, \\ w(L, v) &=& f^-(v), & v < 0\,. \end{array} \right. \tag{57}$$

The recall the definition of the operator $\Theta[V]$, which is non-local in v:

$$\Theta[V] = iV(x + \frac{\partial_v}{2i}) - iV(x - \frac{\partial_v}{2i})\,.$$

For a smooth and decaying potential $V(x)$ it can be rewritten as

$$\Theta[V]w(x, v) = \alpha(x, v) *_v w(x, v), \tag{58}$$

with

$$\alpha(x, v) = \sqrt{\frac{8}{\pi}}\, \Im[e^{2ixv}\, (\mathcal{F}V)(2v)]\,.$$

In order for $\Theta[V]$ to be defined, the potential V has to be given on all of $\mathbb{R}$, although (57) is only posed on the spatial interval $(0, L)$. Again we assume that all constants are normalized: $e = m_* = \hbar = 1$.

As an introduction, we first consider the classical analogue of (57), i.e. the stationary BVP for the Liouville equation:

$$\left\{ \begin{array}{rcll} v f_x - V_x f_x &=& 0, & 0 < x < L, \quad v \in \mathbb{R}\,, \\ f(0, v) &=& f^+(v), & v > 0\,, \\ f(L, v) &=& f^-(v), & v < 0\,. \end{array} \right. \tag{59}$$

As soon as the potential V has a local minimum inside the interval $(0, L)$, (59) has closed characteristic curves (corresponding to particle trajectories). On such closed characteristics, the solution $f(x, v)$ cannot be "controlled" by

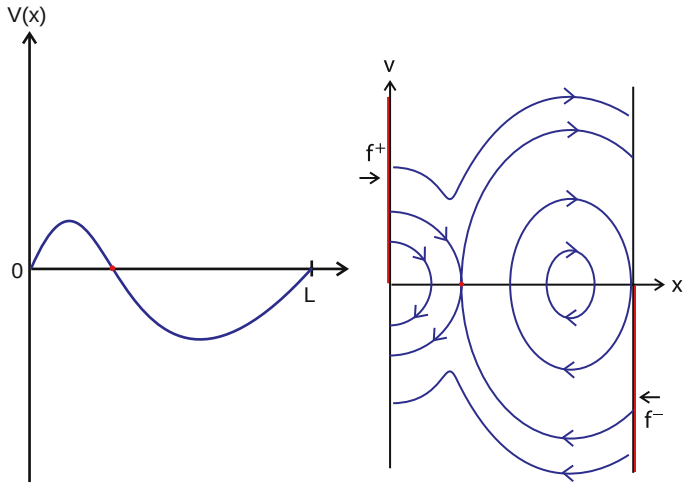

Fig. 10 The given potential $V(x)$ (*left*) gives rise to the phase space trajectories in *right* picture. Note the closed trajectories due to the potential well. There, the solution $f(x,v)$ cannot be "controlled" by the prescribed boundary values f^+, f^-

the boundary values f^+, f^- (cf. Fig. 10). Hence, the solution to (59) is in general non-unique!

For the Wigner equation the picture is very different: Due to the non-locality of $\Theta[V]$), the stationary Wigner equation (57) has *no characteristics* (except for a quadratic potential). Hence, compactly supported steady states cannot exist here (in contrast to the Liouville equation). As we shall see, the stationary solution $w(x,v)$ can be "controlled" by the boundary data.

"Standard" Transport Problems

First we compare (57) to the structure of conventional stationary transport problems, appearing in neutron transport, e.g. [GvMP87]. Those problems are typically of the form

$$vf_x - Af = 0, \qquad 0 < x < L,$$

with a positive Fredholm operator A. The positivity of A reflects the fact, that it models the particle interaction with a diffusive medium.

In the Wigner equation $A(x) := \Theta[V]$ is a skew-symmetric operator on $L^2(\mathbb{R}_v)$. Hence, it does not fall into the above class of standard transport problems.

Discrete Velocity Wigner Model

Since the continuous velocity problem (57) for $vw_x - \Theta[V]w = 0$ is not fully understood yet, we shall discuss here its semi-discretization in velocity. We make the approximation $w_j(x) \approx w(x, v_j)$ with the discrete velocities

$v_1 \geq \cdots \geq v_K > 0 > v_{K+1} \geq \cdots \geq v_N$. Hence, we consider the following BVP for the vector $w(x) \in \mathbb{R}^N$, $x \in [0, L]$:

$$\begin{cases} Tw_x - A(x)w = 0, \quad 0 < x < L\,, \\ w^+(0) = (w_1, \ldots, w_K)^T(x = 0) = f^+\,, \\ w^-(0) = (w_{K+1}, \ldots, w_N)^T(x = L) = f^-\,. \end{cases} \tag{60}$$

Here, T is the diagonal matrix $T = diag(v_1, \ldots, v_N)$. In analogy to $\Theta[V]$, the space-dependent matrix $A(x) \in \mathbb{R}^{N\times N}$ is skew-symmetric $\forall x$. Moreover, $A(x)$ is typically a Toeplitz matrix (in analogy to (58)), but we shall not use this fact below.

Example 7.1. We briefly illustrate, why we exclude here 0 as a discrete velocity. Consider the simple case $N = 3$ with $v_1 = 1$, $v_2 = 0$, $v_3 = -1$. This yields the *algebro-differential equation* (ADE)

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}x} w_1 - \alpha w_2 - \beta w_3 &= 0\,, \\ \alpha w_1 - \gamma w_3 &= 0\,, \\ -\frac{\mathrm{d}}{\mathrm{d}x} w_3 + \beta w_1 + \gamma w_2 &= 0\,, \end{cases} \tag{61}$$

with the (natural) BCs

$$w_1(0) = f^+, \qquad w_3(L) = f^-\,. \tag{62}$$

Since w_2 does not appear in the algebraic constraint (second line of (61)), the index of this ADE is 2. Hence, the BCs (62) make the above system overdetermined and there is either no or infinitely many solutions. This problem of including 0 as a discrete velocity was already observed in numerical discretizations of the stationary Wigner equation [Fre90].

For the analysis of (60) we introduce the transformation: $\tilde{w} = \sqrt{|T|^{-1}} w \quad \in \mathbb{R}^N$. Hence, $Tw_x - A(x)w = 0$ is transformed to

$$\tilde{w}_x - \underbrace{\sqrt{|T|}^{-1} T^{-1} A(x) \sqrt{|T|}}_{:=B(x)} \tilde{w} = 0, \quad x \in (0, L)\,.$$

We make a block decomposition of the matrix $B(x)$ according to the positive and negative velocities v_j:

$$B(x) = \underbrace{\begin{pmatrix} B^{++} & B^{+-} \\ B^{-+} & B^{--} \end{pmatrix}}_{K \quad N-K} \begin{matrix} \}K \\ \}N-K \end{matrix} \begin{matrix} \text{... pos. velocities } v_j \\ \text{... neg. velocities } v_j \end{matrix}$$

These blocks have the following symmetry which is the key structural property for the following theorem:

$$B^{++} = -(B^{++})^T, \quad B^{--} = -(B^{--})^T, \quad B^{+-} = (B^{-+})^T .$$

Theorem 7.1 ([ALZ00]). *Let 0 be none of the discrete velocities, and let* $A \in L^1(0, L; \mathbb{R}^{N\times N})$. *Then, the BVP* (60) *is well-posed.*

Remark 7.2. *In [Fre90] there is numerical evidence of this result.*

Proof. In the discrete velocity BVP $\tilde{w}_x - B(x)\tilde{w} = 0$, the *inflow boundary data* $\tilde{g}^+$, $\tilde{g}^-$ are prescribed. The *outflow boundary data* $\tilde{h}^+$, $\tilde{h}^-$ are obtained from the solution of the problem:

Now we convert the BVP into a forward a backward initial value problem (IVP) with propagator $U(x_1, x_2)$:

$$\begin{pmatrix} \tilde{h}^+ \\ 0 \end{pmatrix} = P^+ \underbrace{U(0,L)}_{\text{propagator}} \begin{pmatrix} \tilde{g}^+ \\ \tilde{h}^- \end{pmatrix}, \quad P^+ = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \tag{63}$$

$$\begin{pmatrix} 0 \\ \tilde{h}^- \end{pmatrix} = P^- \underbrace{U(L,0)}_{=U(0,L)^{-1}} \begin{pmatrix} \tilde{h}^+ \\ \tilde{g}^- \end{pmatrix}, \quad P^- = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}. \tag{64}$$

P^+ and P^- are projection matrices with the same block structure as $B(x)$. Eliminating $\tilde{h}^-$ from these systems yields an equation for the unknown $\tilde{h}^+$:

$$\Big(I \underbrace{-P^+U(0,L)P^-U(L,0)P^+}_{=:K\geq 0}\Big) \begin{pmatrix} \tilde{h}^+ \\ 0 \end{pmatrix}$$

$$= \underbrace{P^+U(0,L)\left[\begin{pmatrix} \tilde{g}^+ \\ 0 \end{pmatrix} + P^-U(L,0)\begin{pmatrix} 0 \\ \tilde{g}^- \end{pmatrix}\right]}_{\text{given}}$$

The matrix K satisfies $K \geq 0$ since $A(x)$ is skew-symmetric. Hence, we can uniquely solve for $\tilde{h}^+$, and the solution $\tilde{w}(x)$ is obtained from a backward problem like (64). □

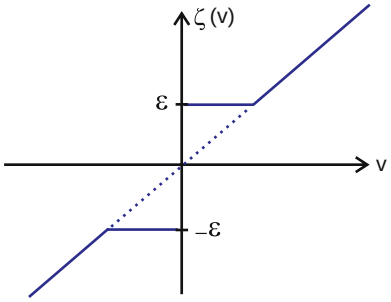

Fig. 11 Velocity cut-off function $\zeta(v)$ for the boundary value problem (65)

A similar strategy gives the following extensions:

- Countably many velocities $v_j \neq 0$.
- Continuous velocity problem ($v \in \mathbb{R}$) with a cut-off for small velocities in the Wigner equation (57) (cf. Fig. 11):

$$\begin{cases} \zeta(v) w_x - \Theta[V]w = 0, & |\zeta| \geq \varepsilon > 0 \\ w(0,v) = f^+; \quad w(L,v) = f^- \end{cases} \tag{65}$$

Theorem 7.3. *Let $V \in L^\infty(\mathbb{R}_x)$, and let the inflow data $f^\pm(v) \in \mathcal{H} := L^2(\mathbb{R}^\pm, |v|\mathrm{d}v)$. Then, the BVP (65) has a unique solution $w \in W^{1,1}((0,L);\mathcal{H})$.*

Proof (idea).

- $V \in L^\infty$ implies $A(x) := \Theta[V] \in L^1((0,L); \mathcal{B}(L^2(\mathbb{R}_v)))$.
- $\frac{1}{\zeta(v)}\Theta[V]$ is a bounded generator for the forward/backward IVP.

□

Remark 7.4. *For the continuous Liouville equation the propagator $U(0,L)$ cannot exist. But Theorem 7.3 applies also to the v-discretized Liouville equation.*

7.2 Exponential Convergence to Steady State

We consider now the time dependent analogue of (60), i.e. the IBVP for the Wigner equation with discrete velocities. We make the approximation $w_j(x,t) \approx w(x,v_j,t)$, $j \in J \subset \mathbb{Z}$. The discrete velocity Wigner function $w(x,t) \in \mathbb{R}^N$ satisfies the following linear hyperbolic system:

$$\begin{cases} w_t + Tw_x - A(x)w = 0, \qquad 0 < x < L, \quad t > 0 \\ w^+(0,t) = f^+;\ w^-(L,t) = f^-, \\ w(x,0) = w^I\,. \end{cases} \tag{66}$$

As before, we assume $T = diag(v_j)_{j\in J}$ and $0 \notin \{v_j\}_{j\in J}$. The matrix $A(x)$ is skew-symmetric for all x and (usually) some v-discretization of the operator $\Theta[V]$.

Theorem 7.5 ([ACT02]). *Let $w^I \in L^2(0,L) \times \ell^2(J)$, $f^\pm \in \mathcal{H} := \ell^2(J;|v_j|)$, and $A \in L^\infty((0,L);\mathcal{B}(\ell^2(J)))$. Then,*

$$w(.,t) \overset{t\to\infty}{\longrightarrow} w_\infty \quad \text{in } L^2(0,L)\times\ell^2(J) \quad \text{with some exponential rate } \varepsilon > 0.$$

w_∞ is the unique steady state of (66), provided by the results of Sect. 7.1.

Remark 7.6. *Since $A(x)$ is skew-symmetric, the system (66) does not show any damping. The exponential decay towards the steady state is only due to outflow through the boundary.*

Proof. Transforming to homogeneous inflow BCs via $\tilde{w} := w - w_\infty$ yields:

$$\begin{cases} \tilde{w}_t + T\tilde{w}_x - A(x)\tilde{w} = 0 \\ \tilde{w}^+(0,t) = 0; \quad \tilde{w}^-(L,t) = 0 \\ \tilde{w}(x,z) = w^I - w_\infty \end{cases} \tag{67}$$

- A naive approach in $L^2(0,L)$ would only yield $\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{w}\|_{L^2(0,L)} \le 0$, but no decay estimate.
- Hence, we shall prove the decay in a weighted L^2-norm. To this end we construct a multiplier matrix $\Phi(x) = diag(\varphi_j(x))_{j\in J}$ with:

$$0 < c \le \varphi_j(x) \le C \qquad \forall j \in J,\ x \in [0,L]$$

- We take the $L^2(0,L)$-inner product of (67) with $\Phi\tilde{w}$. With the notation

$$\|\tilde{w}\|_\Phi^2 := \int_0^L \tilde{w}^\top \cdot \Phi \cdot \tilde{w}\,\mathrm{d}x$$

  we have

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{w}\|_\Phi^2 - \frac{1}{2}\langle\tilde{w}, T\Phi_x\tilde{w}\rangle_{L^2} - \langle A\tilde{w}, \Phi\hat{w}\rangle_{L^2} \le 0\,.$$

  The last inequality is due to outflow at the boundary.
- Now we have to find a matrix function $\Phi(x)$ such that the following inequality holds for some (small) $\varepsilon > 0$:

$$\tfrac{1}{2}\big(f, T\Phi_x(x)f\big) + \big(A(x)f, \Phi(x)f\big) \le -\varepsilon\big(f, \Phi(x)f\big)$$
$$\forall x \in [0,L],\ \forall f \in \mathbb{R}^{|J|}$$

- This holds true, if we have componentwise (i.e. $\forall j \in J$):

$$\frac{1}{2} v_j \frac{\partial}{\partial_x} \varphi_j + \frac{1}{2} \sum_{i \neq j} |a_{ij}(x)||\varphi_i - \varphi_j| \leq -\varepsilon \varphi_j \qquad \text{on } [0, L] \,.$$

- After constructing these functions φ_j, we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\tilde{w}\|_{\Phi} \leq -\varepsilon \|\tilde{w}\|_{\Phi} := -\varepsilon \left\| \sqrt{\varphi_j} \tilde{w}_j(., t) \right\|_{L^2(0,L)} .$$

□

Open Problems

- Removing the velocity cut-off ($\zeta(v) \longrightarrow v$) makes $\frac{1}{\zeta(v)} \Theta[V]$ an unbounded operator in the forward/backward IVPs involved in (63), (64). In this case it is not yet clear how to construct the propagator $U(0, L)$.

- To find conditions on $f^{\pm}$ such that $\hat{\varrho}[w] \geq 0$ or at least $n(x) = \int_{\mathbb{R}} w(x, v) \, \mathrm{d}v \geq 0$ on $[0, L]$ seems to be very difficult. Actually, the Wigner framework is probably not appropriate to answer this question.

- Non-linear (self-consistent) extension of (57):

$$\begin{cases} v w_x - \Theta[V] w &= 0, & 0 < x < L, \quad v \in \mathbb{R} \,, \\ V_{xx} &= D(x) - \int_{\mathbb{R}} w(x, v) \, \mathrm{d}v, & 0 < x < L, \\ w(0, v) &= f^+(v), & v > 0 \,, \\ w(L, v) &= f^-(v), & v < 0 \,. \end{cases}$$

  would need estimates on the quantum-repulsive/attractive potential. Here, some strategies from the stationary quantum-classical coupling in [Ben98] might be extendable.

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