ABOUT A ONE–DIMENSIONAL STATIONARY SCHRÖDINGER–POISSON SYSTEM WITH KOHN–SHAM POTENTIAL

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Abstract

The stationary Schrödinger–Poisson system with a self–consistent effective Kohn–Sham potential is a system of PDEs for the electrostatic potential and the envelopes of wave functions defining the quantum mechanical carrier densities in a semiconductor nanostructure. We regard both Poisson's and Schrödinger's equation with mixed boundary conditions and discontinuous coefficients. Without an exchange–correlation potential the Schrödinger–Poisson system is a nonlinear Poisson equation in the dual of a Sobolev space which is determined by the boundary conditions imposed on the electrostatic potential. The nonlinear Poisson operator involved is strongly monotone and boundedly Lipschitz continuous, hence the operator equation has a unique solution. The proof rests upon the following property: the quantum mechanical carrier density operator depending on the potential of the defining Schrödinger operator is anti–monotone and boundedly Lipschitz continuous. The solution of the Schrödinger–Poisson system without an exchange–correlation potential depends boundedly Lipschitz continuous on the reference potential in Schrödinger's operator. By means of this relation a fixed point mapping for the vector of quantum mechanical carrier densities is set up which meets the conditions in Schauder's fixed point theorem. Hence, the Kohn–Sham system has at least one solution. If the exchange–correlation potential is sufficiently small, then the solution of the Kohn–Sham system is unique. Moreover, properties of the solution as bounds for its values and its oscillation can be expressed in terms of the data of the problem. The one–dimensional case requires special treatment, because in general the physically relevant exchange–correlation potentials are not Lipschitz continuous mappings from the space L^1 into L^2, but into L^1.

Contents

Van Roosbroeck's equations provide a good landscape view on an electronic device, while the Schrödinger–Poisson system portraits the individual features of a nanostructure within the device. In a nanostructure electrons and holes can no longer move freely in all space

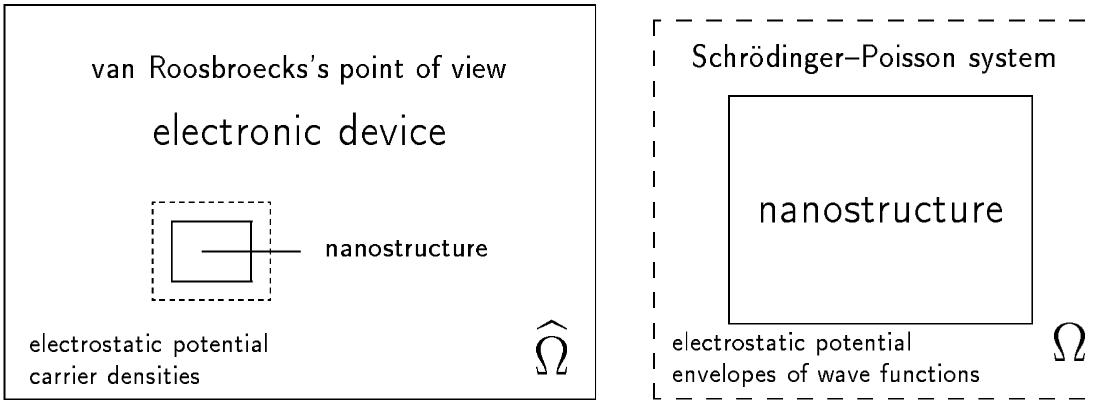

FIGURE 1. Around the nanostructure and beyond

directions and the model of a three–dimensional electron–hole gas is not adequate any more. Instead there is a two–, one– or zero–dimensional electron–hole gas and the densities of electrons and holes have to be computed by quantum mechanical expressions. A suitable model for such a carrier gas with reduced dimension is the Kohn–Sham system i.e. the stationary Schrödinger–Poisson system with a self–consistent effective Kohn–Sham potential (cf. e.g. [2, 8, 19]). From the mathematical point of view this is a system of PDEs for the electrostatic potential and the envelopes of wave functions defining the quantum mechanical carrier densities in the nanostructure. It has to be supplemented by in general mixed boundary conditions (cf. e.g. [7, 8]). For a two–, one– or zero–dimensional carrier gas in a quantum well, quantum wire or quantum dot, the dimension d of the (bounded) spatial domain $\Omega \subset \widehat{\Omega} \subset \mathbb{R}^d$, where we regard the system, is $d = 1, 2, 3$, respectively. In this paper we specifically treat the one–dimensional case ($d = 1$), i.e. quantum well structures, and assume without loss of generality $\Omega = (0, 1) \subset (a, b) = \widehat{\Omega}$. The two– and three–dimensional case will be regarded in a forthcoming paper [13].

The coupling of the nanostructure to its environment is a widely discussed task in modelling and simulation of semiconductor nanostructures (cf. e.g. [7, 19, 20, 21, 3]), but it is open to mathematical validation [11]. The inclusion of the Schrödinger–Poisson system into Van Roosbroeck's equations will be dealt with in this paper only as far as we treat Poisson's equation on the whole device domain thereby assuming given quasi–Fermi potentials on the part of the device domain which is not occupied by the nanostructure. This allows to cope with realistic boundary conditions [8] for the electrostatic potential. In view of modelling equilibrium situations we regard Schrödinger's operator with mixed hard–wall and harmonic boundary conditions. This Schrödinger operator is selfadjoint, has a pure point spectrum, and commutes with the complex conjugation on the underlying Hilbert space. In that case one always finds a complete orthonormal family of real eigenfunctions. Hence the quantum mechanical current vanishes on the whole nanostructure. Even more, the normal derivative of the carrier densities vanishes on the boundary, cf. also §5.b. When leaving equilibrium situations, of course, in general there should be currents over the boundary of the nanostructure [7, 21, 3]. Proper conditions at the interface of the nanostructure and its environment are

- the continuity of each carrier density, and
- the continuity of the normal component of each current.

Aiming at the inclusion of the Schrödinger–Poisson system into Van Roosbroeck's equations one can meet them with a boundary condition for the current continuity equations involving the quantum mechanical carrier densities in addition with the following boundary condition for the Schrödinger operator

$$(*) \qquad \frac{\hbar}{m}\frac{\partial \psi}{\partial \nu} = -\, i\mu\psi\frac{\partial \phi}{\partial \nu} \qquad \text{on } \partial\Omega,$$

where ψ is a state function, m is the effective mass, μ the mobility, and ϕ the quasi–Fermi potential of the carriers under consideration, and ν is the outer unit normal at the boundary $\partial\Omega$ of the nanostructure. If the macroscopic carrier density matches the quantum mechanical carrier density

$$u = \sum_{l=1}^{\infty} N_l |\psi_l|^2,$$

(N_l is the occupation number of the state ψ_l), on the boundary of the nanostructure, then this condition ensures that the normal component of the phenomenological current $-\mu u \operatorname{grad} \phi$ matches the normal component of the quantum mechanical current

$$\frac{\hbar}{m}\sum_{l=1}^{\infty} N_l \Im\left[\psi_l^* \operatorname{grad} \psi_l\right]$$

at the interface. However, the proposed boundary condition makes the corresponding Hamiltonian essentially non–selfadjoint, which leads to the consideration of open quantum systems (cf. [7, 3, 26]). We will treat the inclusion of the Schrödinger–Poisson system into Van Roosbroeck's equations and in particular the Schrödinger operator with the boundary condition $(*)$ in two forthcoming papers [12, 14].

Up to now the mathematical investigation of the Schrödinger–Poisson system has been concentrated on the special case of only one kind of carriers, homogeneous Dirichlet boundary conditions imposed on the electrostatic potential as well as the eigenfunctions of Schrödinger's operator, and without exchange–correlation effects (cf. [6, 23, 24, 25, 8, 1, 15, 16]).

Without an exchange–correlation potential the Schrödinger–Poisson system is a nonlinear Poisson equation in the dual of a Sobolev space which is determined by the boundary conditions imposed on the electrostatic potential. The nonlinear Poisson operator involved is strongly monotone and boundedly Lipschitz continuous, hence the operator equation has a unique solution, and one can establish various methods of descent for its approximative determination [6, 24, 19, 15, 16]. For the method of steepest descent the electrostatic potentials converge uniformly on the device domain which leads to convergence results for the eigenvalues of the corresponding Schrödinger operators [15, 16]. The proof of the stated results on the Schrödinger–Poisson system rests on the following property: the carrier density operator depending on the potential of the defining Schrödinger operator is anti–monotone and boundedly Lipschitz continuous. In establishing this property we rely on form bounds of the Schrödinger operators and on the calculus of double Stieltjes operator integrals [4, 5].

The analytical properties of the Schrödinger–Poisson system pass to the discretized system (cf. [6, 24, 1]), thus allowing proper implementation of the above mentioned iterations, e.g. based on a finite box method as in [9].

If there is an exchange–correlation potential, then the Schrödinger–Poisson system cannot be written anymore as a monotone operator equation neither for the electrostatic potential nor the densities. However, our calculus for the Schrödinger–Poisson system with certain exchange–correlation potentials is based upon the results for the system without exchange–correlation potential inasmuch we freeze the exchange–correlation potential and regard it as a reference potential of a Schrödinger–Poisson systems without exchange–correlation potential. First one can prove that the solution of the Schrödinger–Poisson system without exchange–correlation potential depends boundedly Lipschitz continuous on the reference potential in Schrödinger's operator. By means of this relation a fixed point mapping for the vector of quantum mechanical carrier densities is set up which meets the conditions in Schauder's fixed point theorem. Hence, the Kohn–Sham system has at least one solution. To that end the exchange–correlation potential should be a bounded and continuous mapping of the carrier densities from the space L^1 on a potential from L^1. If the exchange–correlation potential is boundedly Lipschitz continuous and the local Lipschitz constant is sufficiently small, then the solution of the Kohn–Sham system is unique.

In contrast to the cases $d = 2, 3$ in the one–dimensional case ($d = 1$) the physically relevant exchange–correlation potentials in general are not Lipschitz continuous mappings from the space L^1 into L^2, but into L^1. It is due to this fact that we need a calculus for Schrödinger operators with potentials from L^1, and we get it by exploiting the theory of forms. At first we get non–negative carrier densities from the space L^1, which later turn out to be much more regular.

Our present approach to the Kohn–Sham system rests upon the supposed L^1–norm conservation for each kind of carriers. This is a reasonable assumption, as we do not take into account an exchange mechanism of carriers between the nanostructure and the surrounding device within this paper.

In the Schrödinger–Poisson and Kohn–Sham system the electrostatic potential acts via the effective potential in each of the separate scalar Schrödinger equations for electrons and holes. The densities of electrons and holes only couple in Poisson's equation. This approach makes sense for the summary treatment of electrons and holes [17, Appendix A]. For a more detailed investigation of the band structure one has to take into account further band coupling by introducing matrix Schrödinger operators.

1. The one-dimensional Kohn–Sham system

The Kohn–Sham system is a system of equations governing the electrostatic potential φ and the vector $\mathbf{u} = (u_\varsigma)_{\varsigma\in\{1,\ldots,\sigma\}}$ of carrier densities under consideration. Here and in the following the indices $\varsigma \in \{1, \ldots, \sigma\}$ indicate the particle species (electrons and/or holes). The electrostatic potential and the carrier densities have to obey Poisson's equation

$$-\frac{d}{dx}\left(\varepsilon\frac{d}{dx}\varphi\right) = q\Big(N_A - N_D + \sum_{\varsigma\in\{1,\ldots,\sigma\}} e_\varsigma u_\varsigma\Big) \tag{1.1}$$

in the device domain $\widehat{\Omega} = (a, b)$. e_ς is $+1$ for holes and -1 for electrons, q is the magnitude of the elementary charge, and $\varepsilon = \varepsilon(x)$ denotes the dielectric permittivity. The right–hand side of (1.1) is a charge distribution and consists of a fixed density $N_A - N_D$ of ionized dopants and the carrier densities which are defined by the state equations (1.2) and (1.5). Outside the nanostructure there are the state equations

$$u_\varsigma(x) = \mathcal{F}_\varsigma\Big(-e_\varsigma\big(\varphi(x) - \phi_\varsigma(x)\big)\Big) \quad x \in [a,b] \setminus [0,1], \tag{1.2}$$

where we assume that the electrochemical (quasi–Fermi) potentials ϕ_ς are given functions which are fixed throughout this paper. $\mathcal{F}_\varsigma$ are statistical distribution functions. In general there is Fermi–Dirac statistics (cf. e.g. [8]), i.e.

$$\mathcal{F}_\varsigma(\zeta) = c_\varsigma \mathfrak{F}_{\frac{1}{2}}(\zeta), \tag{1.3}$$

where $\mathfrak{F}_\alpha(\zeta)$ denotes Fermi's integral of order α

$$\mathfrak{F}_\alpha(\zeta) = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{\xi^\alpha}{1+\exp(\xi-\zeta)} d\xi \qquad \alpha > -1, \quad \zeta \in \mathbb{R}. \tag{1.4}$$

Inside the nanostructure the carrier densities have to be computed by the quantum mechanical expressions

$$u_\varsigma(\mathfrak{V}_\varsigma)(x) = \sum_{l=1}^{\infty} N_{l,\varsigma}(\mathfrak{V}_\varsigma) \left|\psi_{l,\varsigma}(\mathfrak{V}_\varsigma)(x)\right|^2, \quad x \in \Omega = (0,1), \quad \varsigma \in \{1,\dots,\sigma\}. \tag{1.5}$$

The $N_{l,\varsigma}$ are the occupation factors

$$N_{l,\varsigma}(\mathfrak{V}_\varsigma) = f_\varsigma\left(\mathcal{E}_{l,\varsigma}(\mathfrak{V}_\varsigma) - \mathcal{E}_{F,\varsigma}(\mathfrak{V}_\varsigma)\right), \quad \varsigma \in \{1,\dots,\sigma\}, \tag{1.6}$$

where $\mathcal{E}_{F,\varsigma}$ denotes the Fermi level, and f_ς the thermodynamic equilibrium distribution function of the ς–type carriers.

$\mathcal{E}_{l,\varsigma} = \mathcal{E}_{l,\varsigma}(\mathfrak{V}_\varsigma)$ are the eigenvalues (counting multiplicity) and $\psi_{l,\varsigma} = \psi_{l,\varsigma}(\mathfrak{V}_\varsigma)$ the corresponding orthonormal eigenfunctions of the one–electron Schrödinger operator in effective–mass approximation (Ben–Daniel–Duke form) with the effective Kohn–Sham potential $\mathfrak{V}_\varsigma$

$$\left[-\frac{\hbar^2}{2}\frac{d}{dx}\left(m_\varsigma^{-1}\frac{d}{dx}\right) + \mathfrak{V}_\varsigma\right]\psi_{l,\varsigma} = \mathcal{E}_{l,\varsigma}\psi_{l,\varsigma} \quad \text{in } \Omega = (0,1) \tag{1.7}$$

where $m_\varsigma = m_\varsigma(x)$ is the the position dependent effective–mass of ς–type carriers. The effective Kohn–Sham potentials depend on the carrier densities, and split up in the following way

$$\mathfrak{V}_\varsigma(\mathbf{u}) = -e_\varsigma \Delta E_\varsigma + V_{xc,\varsigma}(\mathbf{u}) + e_\varsigma q \varphi(\mathbf{u})|_{[0,1]}, \tag{1.8}$$

where $\varphi(\mathbf{u})|_{[0,1]}$, denotes the restriction of the electrostatic potential $\varphi(\mathbf{u})$ to the domain $\Omega = (0,1)$ of the nanostructure. The band–edge offsets ΔE_ς are given external potentials representing the electronic characteristics of the material. $V_{xc,\varsigma}$ are the exchange–correlation potentials, which depend on the particle densities. Generic expressions for $V_{xc,\varsigma}$ are

$$V_{xc,\varsigma}(\mathbf{u}) = -\beta_\varsigma u_\varsigma^{\alpha_\varsigma}, \qquad \beta_\varsigma > 0, \quad 0 < \alpha_\varsigma \le 1. \tag{1.9}$$

The Fermi level $\mathcal{E}_{F,\varsigma} = \mathcal{E}_{F,\varsigma}(\mathfrak{V}_\varsigma)$ of the ς–type carriers is defined by the conservation law

$$N_\varsigma = \int_0^1 u_\varsigma(\mathfrak{V}_\varsigma)(x)dx = \sum_{l=1}^{\infty} f_\varsigma\big(\mathcal{E}_{l,\varsigma}(\mathfrak{V}_\varsigma) - \mathcal{E}_{F,\varsigma}(\mathfrak{V}_\varsigma)\big), \tag{1.10}$$

N_ς being the fixed total number of ς–type carriers in the nanostructure domain $\Omega = (0,1)$ under consideration. The distribution functions $f = f_\varsigma$, $\varsigma \in \{1,\dots,\sigma\}$ depend on the reduced dimension of the carrier gas. In the one–dimensional case ($d = 1$) there is

$$f(s) = c\,\mathfrak{F}_0\big(-\frac{s}{\beta}\big) = c\,\ln\Big(1 + \exp\big(-\frac{s}{\beta}\big)\Big), \tag{1.11}$$

with positive constants c and β. The corresponding primitive is

$$F(t) = -\int_t^\infty f(s)ds = -c\beta\,\mathfrak{F}_1\Big(-\frac{t}{\beta}\Big) = -c\beta\,\operatorname{diln}\Big(1+\exp\Big(-\frac{s}{\beta}\Big)\Big), \tag{1.12}$$

and the derivative is

$$f'(s) = -\frac{c}{\beta}\Big(1+\exp\Big(\frac{s}{\beta}\Big)\Big)^{-1}. \tag{1.13}$$

1.1. Remark. The expressions (1.5) and (1.6) apply to electrons as well as to holes, i.e. the energies (and the Fermi level) of quantum mechanical electrons are scaled in the usual way, whereas energies (and the Fermi level) of quantum mechanical holes are counted on a negative energy axis. However, classical electrons and holes both have been treated on the usual energy axis (cf. (1.2)).

In semiconductor device modeling one has to cope in general with rather complex, mixed boundary conditions [8]. As far as the electrostatic potential φ is concerned, we regard the following ones

$$\begin{aligned} \varphi(x) &= \varphi_{\widehat{\Gamma}}(x) && \text{if } x \in \widehat{\Gamma}, \\ -\varepsilon\frac{d}{dx}\varphi(x) &= k\,(\varphi(x) - \varphi_{\widehat{\Gamma}}(x)) && \text{if } x \in \{a,b\}\setminus\widehat{\Gamma}, \end{aligned} \tag{1.14}$$

where the function $\varphi_{\widehat{\Gamma}}$, defined on the closure $[a,b]$ of $\widehat{\Omega}$, represents the boundary values given on $\widehat{\Gamma}$ and the inhomogeneous boundary condition of third kind on $\{a,b\}\setminus\widehat{\Gamma}$. Points from $\widehat{\Gamma}$ model Ohmic contacts, while points from $\{a,b\}\setminus\widehat{\Gamma}$ model interfaces between the semiconductor device and an insulator (with capacity $k \geq 0$) or homogeneous Neumann boundary conditions ($k=0$) (cf. [8]).

It is is a widely discussed question, how to supplement the Schrödinger operators (1.7) by suitable boundary conditions (cf. e.g. [7, 19, 20]. We take into account the following mixed boundary conditions

$$\psi(x) = 0 \quad \text{if } x \in \Gamma, \qquad \frac{d\psi}{dx}(x) = 0 \quad \text{if } x \in \{0,1\}\setminus\Gamma \tag{1.15}$$

for all ψ in the domain of the Schrödinger operator from (1.7). If we assume a device structure which confines the charge carriers, then the carrier densities vanish on the boundary of $\Omega = (0,1)$ and there should be a depletion zone around the nanostructure (cf. [19]). We will prove in §5.b that the boundary conditions (1.15) are compatible with this assumption. We admit mixed boundary conditions in view of modeling cuts through rotational symmetric nanostructures with homogeneous Dirichlet boundary conditions for the eigenfunctions on the physical boundary.

2. Mathematical formulation of the problem

In view of typical applications [8, 9], our mathematical model must necessarily cover semiconductor heterostructures, i.e. the coefficients of Schrödinger's and Poisson's operator are in general discontinuous. This forecloses in particular the domain of the Schrödinger operator lying in $W^{2,2}$, what is commonly used elsewhere, [24, 25, 15]. Fortunately, in the one–dimensional case the $W^{1,2}$–calculus already leads to satisfactory results. In order to represent the homogeneous Dirichlet boundary conditions we have to introduce adequate subspaces of the spaces $\widehat{W^{1,2}} = W^{1,2}(a,b)$ and $W^{1,2} = W^{1,2}(0,1)$.

2.1. Definition. Let $\widehat{\Gamma} \subset \{a, b\}$ and $\Gamma \subset \{0, 1\}$ be the (possibly empty) sets of Dirichlet boundary points of the spatial domains $\widehat{\Omega} = (a, b)$, and $\Omega = (0, 1)$, respectively. We define

$$\begin{aligned} &(2.1) \qquad \widehat{W^{1,2}_{\widehat{\Gamma}}} &= \widehat{W^{1,2}} \cap \{v : v(\widehat{\Gamma}) \subset \{0\}\}, \\ &(2.2) \qquad W^{1,2}_{\Gamma} &= W^{1,2} \cap \{v : v(\Gamma) \subset \{0\}\}, \end{aligned}$$

and denote the corresponding dual spaces by $\widehat{W^{-1,2}_{\widehat{\Gamma}}}$ and $W^{-1,2}_{\Gamma}$, respectively.

2.2. Remark. In the following we will generally index function spaces which refer to the spatial domain $\widehat{\Omega} = (a, b)$ with a hat, while the symbols without a hat are reserved for spaces which refer to the spatial domain $\Omega = (0, 1)$.

Next we introduce a precise notion of the Schrödinger operator.

2.3. Definition. For any $\varsigma \in \{1, \ldots, \sigma\}$ suppose $m = m_\varsigma$ to be in L^∞ with positive values such that m^{-1} is also from L^∞. If V is any real valued function from L^1, then the Schrödinger operator $H_V : W^{1,2}_\Gamma \longmapsto W^{-1,2}_\Gamma$ corresponding to the potential V is defined by

$$\langle H_V v, w \rangle = \frac{\hbar^2}{2} \int_0^1 m(x)^{-1}\, v'(x)\, w'(x) dx + \int_0^1 V(x) v(x) w(x) dx, \quad v, w \in W^{1,2}_\Gamma$$

The definition is justified, because $W^{1,2}_\Gamma$ continuously embeds into L^∞. Thus, the second term on the right hand side of (2.3) is always finite and defines a continuous bilinear form on $W^{1,2}_\Gamma$. In particular, we denote the operator with zero potential by H_0. The restriction of the operators just introduced to other range spaces, in particular L^2, we also denote by H_V.

We notice some properties of the operators H_V which are essentially used in the formulation of the problem and will later be deduced from the results stated in Proposition 3.3.

2.4. Theorem. *For any real valued V from L^1 the restriction of H_V to the range space L^2 is selfadjoint, has a complete orthonormal system of eigenfunctions and all eigenvalues are real.*

About the quasi Fermi potentials, the statistical distribution functions, and the thermodynamic equilibrium distribution functions we assume:

2.5. Assumption. The functions ϕ_ς, which represent the quasi Fermi potentials in (1.2), are from $\widehat{W^{1,2}_{\widehat{\Gamma}}}$.

2.6. Assumption. The statistical distribution functions $\mathcal{F}_\varsigma : \mathbb{R} \longmapsto [0, \infty[$ in (1.2) are monotone and locally Lipschitz continuous. Hence, the mappings $F_\varsigma : \widehat{W^{1,2}_{\widehat{\Gamma}}} \longmapsto \widehat{W^{-1,2}_{\widehat{\Gamma}}}$ which are given by

$$(2.3) \qquad \langle F_\varsigma(v), w \rangle = q \int_{(a,b)\setminus(0,1)} e_\varsigma \mathcal{F}_\varsigma \Big(e_\varsigma \big(\phi_\varsigma(x) - v(x)\big)\Big) w(x)\, dx, \qquad v, w \in \widehat{W^{1,2}_{\widehat{\Gamma}}}.$$

are monotone and locally Lipschitz continuous. Indeed, the Fermi–Dirac distribution function (1.3), which we have mainly in mind, is monotone and locally Lipschitz continuous.

2.7. Assumption. The thermodynamic equilibrium distribution functions $f = f_\varsigma$, $\varsigma \in \{1, \dots, \sigma\}$ from (1.5) are positive, differentiable, strictly monotonously decreasing functions on $\mathbb{R}$. For any $\rho \in \mathbb{R}$ the quantities

$$\sup_{s \in [\frac{1}{2}, \infty[} f(s+\rho)s^3 \quad \text{and} \quad \sup_{s \in [\frac{1}{2}, \infty[} f'(s+\rho)s^4 \tag{2.4}$$

are finite. This assumption covers the distribution functions (1.11).

In applications of the Birman–Solomjak theorem we will frequently encounter the following functions g, which are closely related to the distribution function f.

2.8. Definition. Let f be in accordance with Assumption 2.7, k be one of the numbers 1 or 2, and ρ be an arbitrary real number. We introduce the functions

$$g_{k,\rho} : [0,2] \longmapsto \mathbb{R}, \qquad g_{k,\rho}(t) = \begin{cases} f\left(t^{-1}+\rho\right)t^{-k} & \text{for } s > 0 \\ 0 & \text{for } s = 0 \end{cases} \tag{2.5}$$

and denote by

$$\boldsymbol{L}_{k,\rho} = \sup_{t \in [0,2]} \left| g'_{k,\rho}(t) \right| \tag{2.6}$$

the corresponding Lipschitz constants which are finite by Assumption 2.7, and can easily be expressed in terms of the distribution function f.

2.9. Definition. Let ς be in $\{1, \dots, \sigma\}$, $f = f_\varsigma$ be a distribution function fulfilling Assumption 2.7, and $m = m_\varsigma$ as in Definition 2.3. We define the pseudo carrier density operator corresponding to f and m by

$$\widetilde{\mathcal{N}}(V)(x) = \sum_{l=1}^{\infty} f\big(\mathcal{E}_l(V)\big)\left|\psi_l(V)(x)\right|^2, \quad V \in L^1, \quad x \in [0,1]. \tag{2.7}$$

Here the $\mathcal{E}_l(V)$ and $\psi_l(V)$ are the eigenvalues and L^2–normalized eigenfunctions, respectively, of the Schrödinger operator H_V from Definition 2.3. Further we define the ς–particle density operator $\mathcal{N} = \mathcal{N}_\varsigma$ by

$$\mathcal{N}(V) = \widetilde{\mathcal{N}}\big(V - \mathcal{E}_F(V)\big), \tag{2.8}$$

where $\mathcal{E}_F(V) = \mathcal{E}_{F,\varsigma}(V)$ is the Fermi level defined by

$$\int_0^1 \mathcal{N}(V)\,dx = \sum_l f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) = N, \tag{2.9}$$

$N = N_\varsigma$ being the fixed number of ς–type carriers. We avoid whenever possible the indexing with ς, as in this definition.

2.10. Remark. A priori it is evident only for potentials $V \in L^\infty$ that the Fermi level is well defined, because the spectrum of H_V is then at worst that of H_0, shifted by $-\|V\|_{L^\infty}$. From this, the eigenvalue asymptotics for H_0, the monotonicity and decay properties of the distribution function f follows that $\mathcal{E}_F(V)$ is well defined. This directly implies that the series on the right hand side of (2.7) (there V substituted by $V - \mathcal{E}_F(V)$), which defines the particle density operator $\mathcal{N}_\varsigma$, is absolutely converging in L^1. In Proposition 5.3 we will prove that the particle density operators $\mathcal{N}$ are well defined even as operators from L^1 into spaces of much more regular functions.

2.11. Assumption. The exchange–correlation term in its dependence on the particle densities, i.e. the mapping $\mathbf{u} \longmapsto V_{xc,\varsigma}(\mathbf{u})$ is a continuous and bounded mapping from $\left(L^1\right)^\sigma$ into L^1 for any $\varsigma \in \{1, \dots, \sigma\}$. This assumption covers the generic exchange–correlation potentials (1.9).

2.12. Assumption. The function $\varphi_{\widehat{\Gamma}}$, which represents the boundary values given on $\widehat{\Gamma}$ and the inhomogeneous boundary condition of third kind on $\{a,b\} \setminus \widehat{\Gamma}$ (cf. (1.14)), is from the space $\widehat{W^{1,2}}$. Let $\widetilde{\varphi}_{\widehat{\Gamma}}$ denote the linear form on $\widehat{W^{1,2}_{\widehat{\Gamma}}}$, which is given by

$$h \longmapsto \int_a^b \varepsilon(x)\varphi'_{\widehat{\Gamma}}(x)h'(x)dx, \qquad h \in \widehat{W^{1,2}_{\widehat{\Gamma}}}. \tag{2.10}$$

2.13. Definition. Let the function $\ln\varepsilon(\cdot)$ be from $\widehat{L^\infty}$, and let for any non–Dirichlet boundary point $x \in \{a,b\} \setminus \widehat{\Gamma}$ a positive number $k(x)$ be given. We suppose that either $\widehat{\Gamma}$ is not empty or at least one of the numbers $k(x)$ is strictly positive. The operator $A : \widehat{W^{1,2}_{\widehat{\Gamma}}} \longmapsto \widehat{W^{-1,2}_{\widehat{\Gamma}}}$ is defined by

$$\langle Av, w\rangle = \int_a^b \varepsilon(x)v'(x)w'(x)dx + \sum_{x\in\{a,b\}\setminus\widehat{\Gamma}} k(x)v(x)w(x), \qquad v,w \in \widehat{W^{1,2}_{\widehat{\Gamma}}}.$$

The definition is correct, because $\widehat{W^{1,2}_{\widehat{\Gamma}}}$ embeds continuously into $\widehat{C}$. We denote by c_k a constant such that

$$\|u\|^2_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} \le c_k\Big(\|u'\|^2_{\widehat{L^2}} + \sum_{x\in\{a,b\}\setminus\widehat{\Gamma}} k(x)|u(x)|^2\Big) \qquad \text{for all} \quad u \in \widehat{W^{1,2}_{\widehat{\Gamma}}}. \tag{2.11}$$

The constant c_k depends on (a,b), $\widehat{\Gamma}$ and k. Indeed, it is finite, as the case of purely homogeneous Neumann conditions is excluded [10].

2.14. Definition. Suppose there is

$$N_A - N_D \in \widehat{W^{-1,2}_{\widehat{\Gamma}}}, \qquad \Delta E_\varsigma \in L^1, \qquad \varsigma \in \{1,\dots,\sigma\} \tag{2.12}$$

and a tuple $(Z_1,\dots,Z_\sigma)$ of linear, continuous identification operators

$$Z_\varsigma : \widehat{W^{1,2}} \longmapsto L^1, \qquad \varsigma \in \{1,\dots,\sigma\}. \tag{2.13}$$

Further, let ε, $m_1, \dots, m_\sigma$, $f_1, \dots, f_\sigma$, and $\varphi_{\widehat{\Gamma}}$ be given and the preceding assumptions be satisfied. We define the external potentials V_ς and the effective doping D by

$$V_\varsigma = Z_\varsigma\varphi_{\widehat{\Gamma}} - e_\varsigma \Delta E_\varsigma, \qquad \varsigma \in \{1,\dots,\sigma\}, \tag{2.14}$$

$$D = q(N_A - N_D) - \widetilde{\varphi}_{\widehat{\Gamma}}. \tag{2.15}$$

We say that $(V, u_1, \dots, u_\sigma) \in \widehat{W^{1,2}_{\widehat{\Gamma}}} \times (L^\infty)^\sigma$ is a solution of the Kohn–Sham system (Schrödinger–Poisson system with exchange–correlation potential) if

$$AV = D + \sum_{\varsigma\in\{1,\dots,\sigma\}} Z^*_\varsigma u_\varsigma + F_\varsigma(V), \tag{2.16}$$

$$u_\varsigma = \mathcal{N}_\varsigma\big(V_\varsigma + V_{xc,\varsigma}(\mathbf{u}) + Z_\varsigma V\big), \qquad \varsigma \in \{1,\dots,\sigma\}. \tag{2.17}$$

2.15. Remark. Here and in the sequel we do not formally distinguish between Z_ς and its restriction to the subspace $\widehat{W^{1,2}_{\widehat{\Gamma}}}$. In the same sense Z^*_ς is simultaneously viewed as an operator once into $\widehat{W^{-1,2}}$ and on the other hand, by restriction of the corresponding functionals to $\widehat{W^{1,2}_{\widehat{\Gamma}}}$, into $\widehat{W^{-1,2}_{\widehat{\Gamma}}}$. With respect to the formulation of the problem in §1, the mapping Z_ς is simply the operator, which restricts functions over $[a,b]$ to $[0,1]$, multiplied by $e_\varsigma q$:

$$(Z_\varsigma v)(x) = e_\varsigma q v(x) \quad \text{if } x \in [0,1], \qquad (Z_\varsigma^* w)(x) = \begin{cases} e_\varsigma q w(x) & \text{if } x \in [0,1], \\ 0 & \text{if } x \in [a,b] \setminus [0,1]. \end{cases}$$

However, the authors believe that it can serve well later purpose, to introduce an additional degree of freedom at this point, because the coupling between the macroscopic and the microscopically described part of the device, which expresses here, is by far not completely understood. It turns out that a 'macroscopically extended particle density operator' of the structure described above possesses highly satisfactory functional analytic properties. Even more, as the reader will see in Remark 6.6, the class of admissible operators may be widened by small perturbations.

2.16. Remark. The natural space for the quantum mechanical particle densities u_ς, (2.8), to ly in is L^1, because the conservation laws (2.9) refer to this space. But the functional analytic context, in which we will regard the system, is mainly determined by the monotonicity properties of the nonlinear Poisson operator, acting between $\widehat{W_{\widehat{\Gamma}}^{1,2}}$ and $\widehat{W_{\widehat{\Gamma}}^{-1,2}}$. Thus, we have decided to associate with the notion of a solution that the particle densities are also from L^∞. In fact, it turns out (cf. Remark 6.16) that the structure of the system itself assures that the particle densities are much more regular over $\Omega = (0,1)$, even when at first only $u_\varsigma \in L^1$ is supposed. It should be noted, however, that on the boundary of of $\Omega = (0,1)$ discontinuities of the carrier densities may occur. This is due to the fact that in the present concept the densities u_ς within the quantum mechanically described region $(0,1)$ and in the macroscopically described one are related only via the nonlinear Poisson equation, i.e. the electrostatic potential. A completely self consistent approach would have to include equations for the — macroscopic and microscopic — Fermi potential, a program which we will carry out in later papers [12, 14].

Our approach to the Schrödinger–Poisson system is based upon the following fundamental

2.17. Theorem. *(Cf. e.g. [10].) Let* A *be a strongly monotone and boundedly Lipschitz continuous operator between the Hilbert space* H *and its dual* H^**. The equation*

$$\mathrm{A}(\mathrm{u}) = \mathrm{f} \tag{2.18}$$

admits for any $\mathrm{f} \in H^*$ *exactly one solution. This solution* u *satisfies*

$$\|\mathrm{u}\|_H \le \frac{1}{m_\mathrm{A}} \| \mathrm{A}(0) - \mathrm{f}\|_{H^*}, \tag{2.19}$$

where m_A *denotes the monotonicity constant of* A*. Let* $\mathrm{J} : H \longmapsto H^*$ *be the duality mapping. If* M_A *is the local Lipschitz constant of* A *belonging to a centered ball* K *in* H *with radius not smaller than*

$$\frac{2}{m_\mathrm{A}} \| \mathrm{A}(0) - \mathrm{f}\|_{H^*}, \tag{2.20}$$

then the operator

$$\mathrm{u} \longmapsto \mathrm{u} - \frac{m_\mathrm{A}}{M_\mathrm{A}^2} J^{-1}\big(\mathrm{A}(\mathrm{u}) - \mathrm{f}\big) \tag{2.21}$$

maps the ball K *strictly contractive into itself and its contractivity constant does not exceed*

$$\sqrt{1 - \frac{m_\mathrm{A}^2}{M_\mathrm{A}^2}}. \tag{2.22}$$

The fixed point of (2.21) *is identical with the solution of* (2.18).

Now we recall some properties of the norm in the spaces of q–summable operators.

2.18. Theorem. *Let τ be a positive number, $S = [0, \tau]$, and g a real valued, Lipschitz continuous function on S with $g(0) = 0$. For any selfadjoint, q–summable operator* B*, having its spectrum in S there is*

$$\|g(\mathrm{B})\|_q \leq \mathbf{Lip}_S(g) \, \| \, \mathrm{B} \, \|_q, \tag{2.23}$$

where $\mathbf{Lip}_S(g)$ is the Lipschitz constant of g on S. Moreover, if B *is a q–summable selfadjoint operator, then B^α is $\frac{q}{\alpha}$–summable and*

$$\|\mathrm{B}^\alpha\|_{\frac{q}{\alpha}} = \|\mathrm{B}\|_q^\alpha, \quad 1 \leq q < \infty, \quad 0 < \alpha \leq q. \tag{2.24}$$

2.19. Theorem. *(Birman and Solomjak* [4, 5]*.) Let* A *and* B *be two selfadjoint operators, whose difference is Hilbert–Schmidt and whose spectral measures are concentrated on a finite interval $S \subset \mathbb{R}$. If $g : S \longmapsto \mathbb{R}$ is Lipschitz continuous on S with the Lipschitz constant $\mathbf{Lip}_S(g)$, then*

$$\|g(\mathrm{A}) - g(\mathrm{B})\|_2 \;\leq\; \mathbf{Lip}_S(g) \, \| \, \mathrm{A} - \mathrm{B} \, \|_2. \tag{2.25}$$

3. The Schrödinger operator

In this section we present properties of the Schrödinger operator which are afterwards an essential tool for verifying the existence and uniqueness statements for the Schrödinger–Poisson system. In this section and the two following ones all the function spaces refer to the interval $(0, 1)$. m has to be regarded as any of the effective masses m_ς, $\varsigma \in \{1, \ldots, \sigma\}$. In the following propositions, certain Gagliardo–Nirenberg constants and the L^∞–bound of m play an essential role.

3.1. Definition. We define γ_p as the Gagliardo–Nirenberg constant (cf. e.g. [22])

$$\gamma_1 = \sup_{0 \neq \psi \in W_\Gamma^{1,2}} \frac{\|\psi\|_{L^\infty}}{\sqrt{\|\psi\|_{W_\Gamma^{1,2}} \, \|\psi\|_{L^2}}}, \qquad \gamma_p = \sup_{0 \neq \psi \in W_\Gamma^{1,2}} \frac{\|\psi\|_{L^{\frac{2p}{p-1}}}}{\|\psi\|_{W_\Gamma^{1,2}}^{\frac{1}{2p}} \, \|\psi\|_{L^2}^{1-\frac{1}{2p}}} \quad \text{if } p > 1. \tag{3.1}$$

For any $m = m_\varsigma$, $\varsigma \in \{1, \ldots, \sigma\}$, we denote

$$\overline{m} = \max\left(1, \frac{2\,\|m\|_{L^\infty}}{\hbar^2}\right). \tag{3.2}$$

3.2. Remark. $\overline{m}$ has been defined such that $1/\overline{m}$ is the monotonicity constant of the operator $(H_0 + 1) : W_\Gamma^{1,2} \mapsto W_\Gamma^{-1,2}$, (cf. Definition 2.3), hence, the norm of the inverse operator is not greater than $\overline{m}$:

$$\|\psi\|_{W_\Gamma^{1,2}}^2 \leq \overline{m}\langle (H_0 + 1)\psi, \psi \rangle, \quad \psi \in W_\Gamma^{1,2}, \qquad \left\|(H_0 + 1)^{-1}\right\|_{\mathcal{B}(W_\Gamma^{-1,2}, W_\Gamma^{1,2})} = \overline{m}. \tag{3.3}$$

Further, estimating the eigenvalues of H_0, it is not hard to see that the resolvent of H_0 is nuclear.

Now we regard the Schrödinger operator $H = H_V = H_0 + V$ from Definition 2.3 in the Hilbert space L^2. First, it is standard (cf. Kato [18]) that H_V may also be viewed as the operator, which is induced on L^2 by the form defined in Definition 2.3 if one can show that this form is semibounded and closed. The proof of this is part of the next proposition, which also allows to deduce the statements of Theorem 2.4.

3.3. Proposition. *Let V be real valued and from L^p, $p \in [1, \infty]$.*

i) *If* $\mathfrak{t}$ *is the quadratic form*

$$W^{1,2}_\Gamma \ni \psi \longmapsto \Big\langle (H_0+1)\psi,\bar\psi\Big\rangle = \int_0^1 \frac{1}{m}\psi'\bar\psi' + \psi\bar\psi\,dx, \tag{3.4}$$

and $\mathfrak{t}_V$ *is the quadratic form*

$$W^{1,2}_\Gamma \ni \psi \longmapsto \langle V\psi,\bar\psi\rangle = \int_0^1 V\psi\bar\psi\,dx, \tag{3.5}$$

then for any $\delta>0$ *there is the following form estimate*

$$\begin{aligned}\big|\mathfrak{t}_V[\psi]\big| \;\le\; \mathfrak{t}_{|V|}[\psi] \;\le\; \mathfrak{t}[\psi]^{\frac{1}{2p}}\,\|V\|_{L^p}\,\gamma_p^2\,\overline{m}^{\frac{1}{2p}}\,\big\|\psi\big\|_{L^2}^{2-\frac{1}{p}} \\ \le \frac{\delta}{2p}\mathfrak{t}[\psi] + \delta^{1-2p}\big(1-\frac{1}{2p}\big)\,\big\|V\big\|_{L^p}^{\frac{2p}{2p-1}}\,\gamma_p^{\frac{4p}{2p-1}}\,\overline{m}^{\frac{1}{2p-1}}\,\|\psi\|^2_{L^2}, \quad \psi\in W^{1,2}_\Gamma.\end{aligned} \tag{3.6}$$

ii) *The operator* H_0+V *may be estimated as follows in the sense of forms:*

$$1-\frac{1}{2p}+\rho_V \le \big(1-\frac{1}{2p}\big)(H_0+1)+\rho_V \le\; H_0+V \;\le \big(1+\frac{1}{2p}\big)(H_0+1)-\rho_V-2, \tag{3.7}$$

where

$$\rho_V = -\big(1-\frac{1}{2p}\big)\|V\|_{L^p}^{\frac{2p}{2p-1}}\,\gamma_p^{\frac{4p}{2p-1}}\,\overline{m}^{\frac{1}{2p-1}}-1. \tag{3.8}$$

iii) *If* $\rho\le\rho_V$*, then the spectrum of* $(H_V-\rho)^{-1}$ *is contained in* $[0,2]$ *and*

$$\Big\|(H_V-\rho)^{-\frac12}(H_0+1)^{\frac12}\Big\| = \Big\|(H_0+1)^{\frac12}(H_V-\rho)^{-\frac12}\Big\| \le \big(1-\frac{1}{2p}\big)^{-\frac12}. \tag{3.9}$$

iv) *If* $V\in L^1$ *and* $q\ge1$*, then the resolvent of* H_V *is a* q*–summable operator and*

$$\big\|(H_V-\rho)^{-1}\big\|_q \le \big(1-\frac{1}{2p}\big)^{-1}\big\|(H_0+1)^{-1}\big\|_q<\infty, \qquad \rho\le\rho_V. \tag{3.10}$$

3.4. Remark. (Cf. Kato [18]). The first assertion of Proposition 3.3 says that the form $\mathfrak{t}_V$ is relatively bounded with relative bound zero with respect to the form $\mathfrak{t}$. Hence, the form $\mathfrak{t}+\mathfrak{t}_{V-1}$ is closed and semibounded, thus defining a selfadjoint operator H_V over L^2. The resolvent of this operator is compact, because the resolvent of H_0 is compact. From this the existence of a complete orthonormal system of eigenfunctions follows.

3.5. Remark. The lower form bound of H_0+V in (3.7) can be improved by using the negative part V^- of V instead of $|V|$ to construct the lower bound, i.e. one can replace ρ_V by ρ_{V^-} on the left hand side of (3.7).

Proof of i). We estimate the form $\mathfrak{t}_{|V|}$ by means of Hölder's and the Gagliardo–Nirenberg inequality

$$\Big\langle |V|\psi,\psi\Big\rangle \le \|V\|_{L^p}\|\psi\|^2_{L^{\frac{2p}{p-1}}} \le \|V\|_{L^p}\,\gamma_p^2\,\Big(\|\psi\|^2_{W^{1,2}_\Gamma}\Big)^{\frac{1}{2p}}\,\|\psi\|_{L^2}^{2-\frac1p}$$

and then use (3.3)

$$\le \Big\langle (H_0+1)\psi,\psi\Big\rangle^{\frac{1}{2p}}\,\|V\|_{L^p}\,\gamma_p^2\,\overline{m}^{\frac{1}{2p}}\,\|\psi\|_{L^2}^{2-\frac1p}.$$

Finally we apply Young's inequality. □

Proof of ii). In the sense of forms there is

$$H_0 - |V| \leq H_0 + V \leq H_0 + |V|.$$

Combining this with the first assertion of Proposition 3.3 one obtains (3.7). □

Proof of iii). It suffices to prove the statements for $\rho = \rho_V$, because for $\rho \leq \rho_V$ one has

$$\left\|(H_V - \rho_V)^{\frac{1}{2}}(H_V - \rho)^{-\frac{1}{2}}\right\| \leq 1$$

(cf. [18]). From (3.7) and the definition of ρ_V follows

$$\frac{1}{2}\big(H_0 + 1\big) \leq \big(1 - \frac{1}{2p}\big)\big(H_0 + 1\big) \leq H_V - \rho_V \tag{3.11}$$

in the sense of forms. Consequently, the spectrum of $H_V - \rho_V$ has to ly above $\frac{1}{2}$, and, by the spectral mapping theorem, the spectrum of $(H_V - \rho_V)^{-1}$ is localized in the interval $[0, 2]$. — For $\rho = \rho_V$ (3.9) follows from (3.11), [18, ch. VI, §2], and the fact that the operators $(H_V - \rho)^{-\frac{1}{2}}(H_0 + 1)^{\frac{1}{2}}$ and $(H_0 + 1)^{\frac{1}{2}}(H_V - \rho)^{-\frac{1}{2}}$ are adjoint to each other. □

Proof of iv). (3.10) is trivially implied by (3.9) and the nuclearity of $(H_0 + 1)^{-1}$. □

3.6. Corollary. *From* (3.7) *and the minimax principle (cf. e.g. Reed/Simon* [27]*) one gets the following estimate for the eigenvalues $\mathcal{E}_l(V)$ of the operator $H_V = H_0 + V$:*

$$\big(1 - \frac{1}{2p}\big)(\lambda_l + 1) + \rho_V \leq \mathcal{E}_l(V) \leq \big(1 + \frac{1}{2p}\big)(\lambda_l + 1) - \rho_V - 2, \quad l = 1, 2, \dots, \tag{3.12}$$

where the λ_l are the eigenvalues of the operator H_0, and ρ_V is according to (3.8).

We conclude this section with one more property of the Schrödinger operators from Definition 2.3 with potentials V ranging in a L^1–bounded set $\mathcal{M}$.

3.7. Lemma. *If $\mathcal{M} \subset L^1$ is bounded and*

$$\rho \leq \rho_{\mathcal{M}} = \sup_{V \in \mathcal{M}} \rho_V\big|_{p=1} = -\frac{1}{2}\gamma_1^4 \overline{m} \sup_{V \in \mathcal{M}} \|V\|_{L^1}^2 - 1, \tag{3.13}$$

where $\rho_V|_{p=1}$ is (3.8) *with $p = 1$, and γ_1, $\overline{m}$ are according to Definition 3.1, then the mapping $V \longmapsto (H_V - \rho)^{-1}$ is Lipschitz continuous on $\mathcal{M}$ into the class of Hilbert–Schmidt operators. As a Lipschitz constant one may take*

$$4\,\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2}, L^\infty)}^2 \,\overline{m}\,\left\|(H_0 + 1)^{-1}\right\|_2, \tag{3.14}$$

where $\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2}, L^\infty)}$ is the embedding constant of $W_\Gamma^{1,2}$ into L^∞.

Proof. Obviously there is

$$(H_U - \rho)^{-1} - (H_V - \rho)^{-1} = (H_V - \rho)^{-1}(U - V)(H_U - \rho)^{-1}. \tag{3.15}$$

Taking into account (2.24) and (3.9), one may estimate the Hilbert–Schmidt norm

$$\begin{aligned}
\left\|(H_V - \rho)^{-1}(U - V)(H_U - \rho)^{-1}\right\|_2 &\leq \left\|(H_0 + 1)^{-\frac{1}{2}}\right\|_4 \left\|(H_0 + 1)^{\frac{1}{2}}(H_V - \rho)^{-\frac{1}{2}}\right\| \\
&\quad \cdot \left\|(H_V - \rho)^{-\frac{1}{2}}(U - V)(H_U - \rho)^{-\frac{1}{2}}\right\| \left\|(H_U - \rho)^{-\frac{1}{2}}(H_0 + 1)^{\frac{1}{2}}\right\| \left\|(H_0 + 1)^{-\frac{1}{2}}\right\|_4 \\
&\leq 2\left\|(H_0 + 1)^{-1}\right\|_2 \left\|(H_V - \rho)^{-\frac{1}{2}}(U - V)(H_U - \rho)^{-\frac{1}{2}}\right\|.
\end{aligned}$$

Further, the last factor on the right hand side of this inequality can be estimated by means of (3.9):

$$
\begin{aligned}
(3.16)\qquad \left\|(H_V-\rho)^{-\frac{1}{2}}(U-V)(H_V-\rho)^{-\frac{1}{2}}\right\| \;&\le\; \left\|(H_V-\rho)^{-\frac{1}{2}}(H_0+1)^{\frac{1}{2}}\right\| \\
&\quad\cdot \left\|(H_0+1)^{-\frac{1}{2}}(U-V)(H_0+1)^{-\frac{1}{2}}\right\| \left\|(H_0+1)^{\frac{1}{2}}(H_U-\rho)^{-\frac{1}{2}}\right\| \\
&\le 2\left\|(H_0+1)^{-\frac{1}{2}}\right\|_{\mathcal{B}(L^1,L^2)}\left\|U-V\right\|_{L^1}\left\|(H_0+1)^{-\frac{1}{2}}\right\|_{\mathcal{B}(L^2,L^\infty)} \\
&\le 2\left\|(H_0+1)^{-\frac{1}{2}}\right\|^2_{\mathcal{B}(L^2,L^\infty)}\left\|U-V\right\|_{L^1} \;\le\; 2\,\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\,\|U-V\|_{L^1}.
\end{aligned}
$$

The last step in the estimate (3.16) follows from

$$
(3.17)\qquad \left\|(H_0+1)^{-\frac{1}{2}}\right\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)} = \left\|(H_0+1)^{-1}\right\|^{\frac{1}{2}}_{\mathcal{B}(W^{-1,2}_\Gamma,W^{1,2}_\Gamma)} \le \overline{m}^{\frac{1}{2}}
$$

(cf. Remark 3.2). □

4. The Fermi level

In this section and the following one we develop some tools which we need for the existence proof. Partly, these results have already been proved in the case of pure Dirichlet boundary conditions. Here we present proofs, however, which are quite different in character. They completely avoid the Dunford calculus employed in [15] and use the embedding of the eigenvalues of H_0+V, given by Corollary 3.6, or the Birman–Solomjak theorem instead. Thus, we get a priori bounds for the Fermi level and for the solutions in terms of the data of the problem.

First we state a lemma, the proof of which exemplifies the way we estimate functions of the Schrödinger operator.

4.1. Lemma. *Let $\mathcal{M}\subset L^1$ be bounded, f be a distribution function as in Assumption 2.7, and H_V be the Schrödinger operator from Definition 2.3. The mapping $V\longmapsto f(H_V)$ is Lipschitz continuous on $\mathcal{M}$ into the class of nuclear operators, more precisely, for any two elements U,V of $\mathcal{M}$, there is*

$$
\left\|f(H_U)-f(H_V)\right\|_1 \le 16\,\boldsymbol{L}_{1,\rho_\mathcal{M}}\,\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\,\overline{m}\,\left\|(H_0+1)^{-1}\right\|_2^2\|U-V\|_{L^1},
$$

where $\boldsymbol{L}_{1,\rho_\mathcal{M}}$ is the Lipschitz constant from Definition 2.8, and $\rho_\mathcal{M}$ is the number (3.13).

Proof. We abbreviate $\rho=\rho_\mathcal{M}$. First we observe

$$
\begin{aligned}
(4.1)\qquad \left\|f(H_U)-f(H_V)\right\|_1 \le &\left\|f(H_U)(H_U-\rho)\right\|_2\left\|(H_U-\rho)^{-1}-(H_V-\rho)^{-1}\right\|_2 \\
&+\left\|f(H_U)(H_U-\rho)-f(H_V)(H_V-\rho)\right\|_2\left\|(H_V-\rho)^{-1}\right\|_2.
\end{aligned}
$$

In order to estimate the terms

$$
\left\|f(H_U)(H_U-\rho)\right\|_2 \qquad\text{and}\qquad \left\|f(H_U)(H_U-\rho)-f(H_V)(H_V-\rho)\right\|_2
$$

by means of Theorem 2.18 and the Birman–Solomjak Theorem 2.19 we rewrite for $W\in\mathcal{M}$

$$
f(H_W)(H_W-\rho)=g\big((H_W-\rho)^{-1}\big),
$$

where $g=g_{1,\rho}$ is the function (2.5). Indeed, this is justified by Proposition 3.3, which states that the spectrum of $(H_W-\rho)^{-1}$ is contained in $[0,2]$ for all $W\in\mathcal{M}$. Consequently Theorem 2.18 yields

$$
\left\|f(H_U)(H_U-\rho)\right\|_2 = \left\|g\big((H_U-\rho)^{-1}\big)\right\|_2 \le \boldsymbol{L}_{1,\rho}\left\|(H_U-\rho)^{-1}\right\|_2.
$$

Correspondingly we get with Theorem 2.19

$$\begin{aligned}&\big\|f(H_U)(H_U-\rho)-f(H_V)(H_V-\rho)\big\|_2\\&\qquad=\big\|g((H_U-\rho)^{-1})-g((H_V-\rho)^{-1})\big\|_2\le \boldsymbol{L}_{1,\rho}\,\big\|(H_U-\rho)^{-1}-(H_V-\rho)^{-1}\big\|_2.\end{aligned}$$

Hence (4.1) may be majorized by

$$\boldsymbol{L}_{1,\rho}\left(\big\|(H_U-\rho)^{-1}\big\|_2+\big\|(H_V-\rho)^{-1}\big\|_2\right)\left\|(H_U-\rho)^{-1}-(H_V-\rho)^{-1}\right\|_2.$$

Now one can estimate $\|(H_U-\rho)^{-1}\|_2$ and $\|(H_V-\rho)^{-1}\|_2$ by means of (3.10), and the term $\|(H_U-\rho)^{-1}-(H_V-\rho)^{-1}\|_2$ by means of Lemma 3.7 using the Lipschitz constant (3.14). □

4.2. Proposition. *Let $\varsigma\in\{1,\dots,\sigma\}$ be arbitrary, H_V be the Schrödinger operator from Definition 2.3 and $\mathcal{E}_F=\mathcal{E}_{F,\varsigma}$ be the Fermi level from Definition 2.9.*

i) *If $V\in L^1$ and $U\in L^\infty$, then*

$$|\mathcal{E}_F(V+U)-\mathcal{E}_F(V)|\le\|U\|_{L^\infty}. \tag{4.2}$$

ii) *Let $\{\lambda_l\}$ be the sequence of eigenvalues of the free Hamiltonian H_0. We define for any $p\ge1$ the numbers $\underline{\epsilon}_p$ and $\bar{\epsilon}_p$ by*

$$\sum_{l=1}^{\infty}f\Big(\big(1-\frac{1}{2p}\big)\lambda_l-\underline{\epsilon}_p\Big)\;=\;\sum_{l=1}^{\infty}f\Big(\big(1+\frac{1}{2p}\big)\lambda_l-\bar{\epsilon}_p\Big)\;=\;N, \tag{4.3}$$

where N is as in (2.9). If $p\ge1$ and $V\in L^p$, then one has the following bounds for the Fermi level $\mathcal{E}_F(V)$:

$$\underline{\epsilon}_p+\rho_V+\big(1-\frac{1}{2p}\big)\;\le\;\mathcal{E}_F(V)\;\le\;\bar{\epsilon}_p-\rho_V-\big(1-\frac{1}{2p}\big), \tag{4.4}$$

where ρ_V is as in (3.8).

iii) *$V\longmapsto\mathcal{E}_F(V)$ is a locally Lipschitz continuous mapping $\mathcal{E}_F:L^1\longmapsto\mathbb{R}$, more precisely, if $\mathcal{M}$ is a bounded subset of L^1, and $\rho=\rho_{\mathcal{M}+\mathcal{E}_F(\mathcal{M})\chi_{[0,1]}}$ is the number (3.13) corresponding to the set $\mathcal{M}+\mathcal{E}_F(\mathcal{M})\chi_{[0,1]}$, where $\chi_{[0,1]}$ is the characteristic function of the interval $\Omega=(0,1)$, then*

$$\mathbf{Lip}_{\mathcal{M}}(\mathcal{E}_F)=16\,\delta_{\mathcal{M}}\,\boldsymbol{L}_{1,\rho}\,\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\,\overline{m}\,\big\|(H_0+1)^{-1}\big\|_2^2 \tag{4.5}$$

is a Lipschitz constant of $\mathcal{E}_F$ on $\mathcal{M}$. $\boldsymbol{L}_{1,\rho}$ is from Definition 2.8.

Proof of i). (4.2) follows from the strict decay of f (cf. Assumption 2.7) and the form inequality

$$H_V\le H_{V+U}+\|U\|_{L^\infty},$$

which implies a corresponding inequality for the eigenvalues. □

Proof of ii). We prove the left part of (4.4), the other part runs along the same lines. Assume the opposite, namely

$$\underline{\epsilon}_p+\rho_V+\big(1-\frac{1}{2p}\big)>\mathcal{E}_F(V).$$

This implies in connection with the left part of the eigenvalue inequality (3.12) and the strict decay of the distribution function f

$$f\Big(\big(1-\frac{1}{2p}\big)\lambda_l-\underline{\epsilon}_p\Big)<f\Big(\mathcal{E}_l(V)-\mathcal{E}_F(V)\Big)$$

which contradicts the definitions (4.3) and (1.10) of $\underline{\epsilon}_p$ and $\mathcal{E}_F(V)$, respectively. □

Proof of iii). If U, V are two elements of $\mathcal{M}$, then we may estimate

$$(4.6)\quad \left|\mathcal{E}_F(U) - \mathcal{E}_F(V)\right| \le \delta_{\mathcal{M}} \left| f\big(\mathcal{E}_1(V) - \mathcal{E}_F(V)\big) - f\big(\mathcal{E}_1(V) - \mathcal{E}_F(U)\big)\right|,$$

where $\delta_{\mathcal{M}} =$

$$\sup_{U,V\in\mathcal{M}} \sup \left\{ \frac{1}{|f'(s)|} \;:\; \min\{\mathcal{E}_F(V), \mathcal{E}_F(U)\} \le \mathcal{E}_1(V) - s \le \max\{\mathcal{E}_F(V), \mathcal{E}_F(U)\} \right\}.$$

$\delta_{\mathcal{M}}$ can be estimated using the bounds for $\mathcal{E}_1(V)$ established in Corollary 3.6 and the bounds (4.4) for the Fermi levels $\mathcal{E}_F(U), \mathcal{E}_F(V)$. From this and the supposed properties of the distribution function f (cf. Assumption 2.7) follows that $\delta_{\mathcal{M}}$ is finite.

Observing that according to (2.9)

$$N = \operatorname{tr}\big[f(H_V - \mathcal{E}_F(V))\big] = \operatorname{tr}\big[f(H_U - \mathcal{E}_F(U))\big],$$

we continue (4.6) by further enlarging the right hand side

$$\begin{aligned}
\left|\mathcal{E}_F(U) - \mathcal{E}_F(V)\right| &\le \delta_{\mathcal{M}} \left| f\big(\mathcal{E}_1(V) - \mathcal{E}_F(V)\big) - f\big(\mathcal{E}_1(V) - \mathcal{E}_F(U)\big)\right| \\
&\le \delta_{\mathcal{M}} \left| \operatorname{tr}\Big[f\big(H_V - \mathcal{E}_F(V)\big) - f\big(H_V - \mathcal{E}_F(U)\big)\Big]\right| \\
&\le \delta_{\mathcal{M}} \left\| f\big(H_{U-\mathcal{E}_F(U)}\big) - f\big(H_{V-\mathcal{E}_F(U)}\big)\right\|_1 \\
&\le 16\, \delta_{\mathcal{M}}\, \boldsymbol{L}_{1,\rho} \, \|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma, L^\infty)}\, \overline{m}\, \left\|(H_0+1)^{-1}\right\|_2^2 \|U - V\|_{L^1},
\end{aligned}$$

where the last estimate follows from Lemma 4.1. N.B. the set $\mathcal{M}+\mathcal{E}_F(\mathcal{M})\chi_{[0,1]}$, is bounded due to (4.4). □

5. The particle density operator

This section deals with a priori estimates, Lipschitz properties and the boundary behaviour of the particle density operators $\mathcal{N}_\varsigma$. We will use these results in the existence proof.

5.a. **A priori estimates and Lipschitz continuity.** In this subsection we will derive estimates of the carrier density operators and corresponding Lipschitz constants. One cornerstone is a representation formula, which expresses the duality between a value of the particle density operator and a L^∞–function. It has been introduced into the theory of the Schrödinger–Poisson system by F. Nier in his pioneering papers [23, 25].

5.1. Theorem. *If $U \in L^\infty$ and $W \in L^\infty$, then the duality between $\widetilde{\mathcal{N}}(U) \in L^1$ (cf. Definition 2.9) and W can be written as*

$$(5.1)\qquad \langle \widetilde{\mathcal{N}}(U), W\rangle = \int_0^1 \widetilde{\mathcal{N}}(U)(x) W(x)\, dx \;=\; \operatorname{tr}\big[f(H_U)W\big].$$

5.2. Remark. Formula (5.1) extends canonically to potentials U from L^1, because the mapping $U \longmapsto f(H_U)$ is a continuous mapping from L^1 into the class of nuclear operators (cf. Lemma 4.1). In particular, if $U = V - \mathcal{E}_F(V)$, where $\mathcal{E}_F(V)$ is again the Fermi level corresponding to the potential V (cf. Definition 2.9), then

$$(5.2)\qquad \langle \mathcal{N}(V), W\rangle = \int_0^1 \widetilde{\mathcal{N}}\big(V - \mathcal{E}_F(V)\big)(x) W(x)\, dx \;=\; \operatorname{tr}\Big[f\big(H_{V-\mathcal{E}_F(V)}\big)W\Big].$$

This formula allows to define particle density operators also in contexts, where the Fermi level is given otherwise (e.g. externally) and needs not be a constant.

5.3. Proposition. *Let $\mathcal{N}$ be the carrier density operator from Definition 2.9. The operator $V \longmapsto \mathcal{N}(V) = \widetilde{\mathcal{N}}\big(V - \mathcal{E}_F(V)\big)$ is not only well defined as an operator from L^1 into itself, but takes its values in $W^{1,2}_\Gamma$. If $\mathcal{M}$ is a bounded subset of L^1, and $\rho \le \rho_{\mathcal{M}}$ is as in* (3.13)*, then*

$$(5.3) \qquad \big\|\mathcal{N}(V)\big\|_{W^{1,2}_\Gamma} \le 8\,\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma, L^\infty)}\overline{m}\,\big\|(H_0+1)^{-1}\big\|_1 \sup_{s\ge\frac{1}{2}} f\big(s - \bar{\epsilon}_1 + 2\rho + \frac{1}{2}\big)s^2,$$

where $\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma, L^\infty)}$ again denotes the embedding constant from $W^{1,2}_\Gamma$ into L^∞.

The pseudo particle density operator $\widetilde{\mathcal{N}} : L^1 \longmapsto W^{1,2}_\Gamma$ from Definition 2.9 is locally Lipschitz continuous, more precisely

$$(5.4) \qquad \big\|\widetilde{\mathcal{N}}(U) - \widetilde{\mathcal{N}}(V)\big\|_{W^{1,2}_\Gamma} \le 96\,\overline{m}^2\,\boldsymbol{L}_{2,\rho}\,\|\mathbb{1}\|^3_{\mathcal{B}(W^{1,2}_\Gamma, L^\infty)}\big\|(H_0+1)^{-1}\big\|_2^2\|U - V\|_{L^1},$$

where $\boldsymbol{L}_{2,\rho}$ is the Lipschitz constant (2.6).

Proof of (5.3). We introduce the set

$$(5.5) \qquad K = \big\{W \in L^\infty : \|W\|_{W^{-1,2}_\Gamma} = 1\big\}.$$

From the density of L^∞ in $W^{-1,2}_\Gamma$ easily follows for all V from L^1

$$(5.6) \qquad \big\|\mathcal{N}(V)\big\|_{W^{1,2}_\Gamma} = \sup_{\|W\|_{W^{-1,2}_\Gamma}=1} \Big|\big\langle \mathcal{N}(V), W\big\rangle\Big| = \sup_{W\in K}\Big|\big\langle \mathcal{N}(V), W\big\rangle\Big|$$

and by Theorem 5.1

$$(5.7) \quad \big\|\mathcal{N}(V)\big\|_{W^{1,2}_\Gamma} = \sup_{W\in K}\left|\operatorname{tr}\Big[f\big(H_V - \mathcal{E}_F(V)\big)W\Big]\right|$$
$$\le \Big\|f\big(H_V - \mathcal{E}_F(V)\big)(H_V-\rho)^2\Big\|\,\big\|(H_V-\rho)^{-1}\big\|_1\,\big\|(H_V-\rho)^{-\frac{1}{2}}W(H_V-\rho)^{-\frac{1}{2}}\big\|.$$

Taking into account the estimate (4.4) for the Fermi levels, one obtains

$$\Big\|f\big(H_V - \mathcal{E}_F(V)\big)(H_V-\rho)^2\Big\| \le \sup_{s\ge\frac{1}{2}} f\big(s - \bar{\epsilon}_1 + 2\rho + \frac{1}{2}\big)s^2.$$

According to Corollary 3.6 and (3.13) there is

$$\big\|(H_V-\rho)^{-1}\big\|_1 \le 2\,\big\|(H_0+1)^{-1}\big\|_1.$$

It remains to estimate the last factor in (5.7):

$$\sup_{W\in K}\big\|(H_V-\rho)^{-\frac{1}{2}}W(H_V-\rho)^{-\frac{1}{2}}\big\| \le 2\sup_{W\in K}\big\|(H_0+1)^{-\frac{1}{2}}W(H_0+1)^{-\frac{1}{2}}\big\|$$
$$= 2\sup_{W\in K}\sup_{\|\psi\|_{L^2}=\|\tilde{\psi}\|_{L^2}=1}\Big|\big\langle (H_0+1)^{-\frac{1}{2}}W(H_0+1)^{-\frac{1}{2}}\psi, \tilde{\psi}\big\rangle\Big|.$$

Let W be from K, and $\psi, \tilde{\psi}$ from the unit sphere of L^2. The selfadjointness of H_0 provides

$$\Big|\big\langle (H_0+1)^{-\frac{1}{2}}W(H_0+1)^{-\frac{1}{2}}\psi, \tilde{\psi}\big\rangle\Big| = \Big|\big\langle W(H_0+1)^{-\frac{1}{2}}\psi, (H_0+1)^{-\frac{1}{2}}\tilde{\psi}\big\rangle\Big|.$$

The duality between $W^{1,2}_\Gamma$ and $W^{-1,2}_\Gamma$ coincides with the $\big(L^1, L^\infty\big)$–duality on the common intersection of the dual pairs, hence, we may continue

$$\begin{aligned}
&\le\ \|W\|_{W^{-1,2}_\Gamma} \left\| \left((H_0+1)^{-\frac12}\psi\right)\left((H_0+1)^{-\frac12}\tilde\psi\right)^*\right\|_{W^{1,2}_\Gamma}\\
&\le\ \big\|(H_0+1)^{-\frac12}\psi\big\|_{L^\infty}\big\|(H_0+1)^{-\frac12}\tilde\psi\big\|_{W^{1,2}_\Gamma} + \big\|(H_0+1)^{-\frac12}\psi\big\|_{W^{1,2}_\Gamma}\big\|(H_0+1)^{-\frac12}\tilde\psi\big\|_{L^\infty}\\
&\le\ 2\,\|(H_0+1)^{-\frac12}\|_{\mathcal{B}(L^2,L^\infty)}\|(H_0+1)^{-\frac12}\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)}\ \le\ 2\,\|\mathbb{1}\|_{\mathcal{B}\left(W^{1,2}_\Gamma,L^\infty\right)}\,\overline{m}.
\end{aligned}$$

The assertion that $\mathcal{N} : L^1 \mapsto L^1$ is well defined follows from (5.3) and the embedding $W^{1,2}_\Gamma \hookrightarrow L^1$. □

Proof of (5.4). According to Theorem 5.1 there is

$$\big\|\widetilde{\mathcal{N}}(U) - \widetilde{\mathcal{N}}(V)\big\|_{W^{1,2}_\Gamma} = \sup_{W\in K}\Big|\operatorname{tr}\big[\big(f(H_U)-f(H_V)\big)W\big]\Big|$$

which we can estimate as follows

$$\begin{aligned}
&\le \sup_{W\in K}\left|\operatorname{tr}\Big[\Big(f(H_U)(H_U-\rho)^2 - f(H_V)(H_V-\rho)^2\Big)(H_U-\rho)^{-1}W(H_U-\rho)^{-1}\Big]\right|\\
&\quad+\sup_{W\in K}\left|\operatorname{tr}\Big[f(H_V)(H_V-\rho)^2\Big((H_U-\rho)^{-1}W(H_U-\rho)^{-1} - (H_V-\rho)^{-1}W(H_V-\rho)^{-1}\Big)\Big]\right|\\
&\le \big\|f(H_U)(H_U-\rho)^2 - f(H_V)(H_V-\rho)^2\big\|_2 \sup_{W\in K}\big\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1}\big\|_2\\
&\quad+\big\|f(H_V)(H_V-\rho)^2\big\|_2 \sup_{W\in K}\big\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1} - (H_V-\rho)^{-1}W(H_V-\rho)^{-1}\big\|_2.
\end{aligned}$$

Observing the Definition 2.8 of $\boldsymbol{L}_{2,\rho}$, Theorem 2.18 and (3.10) one obtains

$$\big\|f(H_V)(H_V-\rho)^2\big\|_2 \le\ \boldsymbol{L}_{2,\rho}\,\big\|(H_V-\rho)^{-1}\big\|_2 \le\ 2\,\boldsymbol{L}_{2,\rho}\,\big\|(H_0+1)^{-1}\big\|_2,$$

while the Birman–Solomjak Theorem 2.19 and Lemma 3.7 yield

$$\begin{aligned}
\big\|f(H_U)(H_U-\rho)^2 - f(H_V)(H_V-\rho)^2\big\|_2 &\le \boldsymbol{L}_{2,\rho}\,\big\|(H_U-\rho)^{-1} - (H_V-\rho)^{-1}\big\|_2\\
&\le 4\,\boldsymbol{L}_{2,\rho}\,\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\,\overline{m}\,\big\|(H_0+1)^{-1}\big\|_2\,\|U-V\|_{L^1}.
\end{aligned}$$

Now we will treat the terms with $(H_U-\rho)^{-1}W(H_U-\rho)^{-1}$:

$$\begin{aligned}
&\Big\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1} - (H_V-\rho)^{-1}W(H_V-\rho)^{-1}\Big\|_2\\
&\quad\le\ \Big\|\Big((H_V-\rho)^{-1}(V-U)(H_U-\rho)^{-1}\Big)W(H_U-\rho)^{-1}\Big\|_2\\
&\qquad+\Big\|(H_V-\rho)^{-1}W\Big((H_V-\rho)^{-1}(V-U)(H_U-\rho)^{-1}\Big)\Big\|_2\\
&\quad\le\ \big\|(H_V-\rho)^{-\frac12}(H_0+1)^{\frac12}\big\|\,\big\|(H_0+1)^{-\frac12}\big\|_4\,\big\|(H_V-\rho)^{-\frac12}(V-U)(H_U-\rho)^{-\frac12}\big\|\\
&\qquad\quad\cdot\big\|(H_U-\rho)^{-\frac12}W(H_U-\rho)^{-\frac12}\big\|\,\big\|(H_U-\rho)^{-\frac12}(H_0+1)^{\frac12}\big\|\,\big\|(H_0+1)^{-\frac12}\big\|_4\\
&\qquad+\big\|(H_V-\rho)^{-\frac12}(H_0+1)^{\frac12}\big\|\,\big\|(H_0+1)^{-\frac12}\big\|_4\,\big\|(H_V-\rho)^{-\frac12}W(H_V-\rho)^{-\frac12}\big\|\\
&\qquad\quad\cdot\big\|(H_V-\rho)^{-\frac12}(V-U)(H_U-\rho)^{-\frac12}\big\|\,\big\|(H_U-\rho)^{-\frac12}(H_0+1)^{\frac12}\big\|\,\big\|(H_0+1)^{-\frac12}\big\|_4.
\end{aligned}$$

We continue by enlarging

$$\big\|(H_U-\rho)^{-\frac12}(H_0+1)^{\frac12}\big\| \le \sqrt{2}\quad\text{and}\quad\big\|(H_V-\rho)^{-\frac12}(H_0+1)^{\frac12}\big\| \le \sqrt{2}$$

(cf. (3.9)) and estimating the term

$$\big\|(H_V-\rho)^{-\frac12}(V-U)(H_U-\rho)^{-\frac12}\big\|$$

in the same way as in (3.16). Thus, one obtains

$$\begin{aligned}
&\left\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1}-(H_V-\rho)^{-1}W(H_V-\rho)^{-1}\right\|_2\\
&\quad\le 8\left\|(H_0+1)^{-1}\right\|_2\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\,\|U-V\|_{L^1}\left\|(H_V-\rho)^{-\frac12}W(H_V-\rho)^{-\frac12}\right\|\\
&\qquad\le 16\left\|(H_0+1)^{-1}\right\|_2\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\,\|U-V\|_{L^1}\left\|(H_0+1)^{-\frac12}W(H_0+1)^{-\frac12}\right\|.
\end{aligned}$$

Similarly, one proves

$$\begin{aligned}
\left\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1}\right\|_2 \;\le\; 2\left\|(H_0+1)^{-\frac12}\right\|_4^2\left\|(H_V-\rho)^{-\frac12}W(H_V-\rho)^{-\frac12}\right\|\\
\le 4\left\|(H_0+1)^{-1}\right\|_2\left\|(H_0+1)^{-\frac12}W(H_0+1)^{-\frac12}\right\|.
\end{aligned}$$

Now we assemble our estimates

$$\begin{aligned}
&\left\|\widetilde{\mathcal{N}}(U)-\widetilde{\mathcal{N}}(V)\right\|_{W^{1,2}_\Gamma}\\
&\le 48\,\overline{m}\,\boldsymbol{L}_{2,\rho}\,\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\left\|(H_0+1)^{-1}\right\|_2^2\|U-V\|_{L^1}\sup_{W\in K}\left\|(H_0+1)^{-\frac12}W(H_0+1)^{-\frac12}\right\|,
\end{aligned}$$

and observe that the last factor has already been estimated in the proof of (5.3). □

The following two corollaries result directly from Definition 2.9, Proposition 4.2, and Proposition 5.3.

5.4. Corollary. *The mappings $\mathcal{N}_\varsigma : L^1 \longmapsto W^{1,2}_\Gamma$, $\varsigma \in \{1,\dots,\sigma\}$, are locally Lipschitz continuous. If $\mathcal{M}$ is a bounded set from L^1, then the Lipschitz constant of $\mathcal{N}_\varsigma$ on $\mathcal{M}$ is*

$$\mathbf{Lip}_{\mathcal{M}}(\mathcal{N}_\varsigma)\le\Big(1+\mathbf{Lip}_{\mathcal{M}}(\mathcal{E}_{F,\varsigma})\Big)\mathbf{Lip}_{\left(\mathcal{M}+\mathcal{E}_{F,\varsigma}(\mathcal{M})\chi_{[0,1]}\right)}(\widetilde{\mathcal{N}}_\varsigma),$$

where $\mathbf{Lip}_{\mathcal{M}}(\mathcal{E}_{F,\varsigma})$ is the Lipschitz constant of the Fermi level $\mathcal{E}_{F,\varsigma}$ on the set $\mathcal{M}$, cf. (4.5), and $\mathbf{Lip}_{\left(\mathcal{M}+\mathcal{E}_{F,\varsigma}(\mathcal{M})\chi_{[0,1]}\right)}(\widetilde{\mathcal{N}}_\varsigma)$ is the Lipschitz constant of $\widetilde{\mathcal{N}}_\varsigma : L^1 \longmapsto W^{1,2}_\Gamma$ on the bounded set $\mathcal{M}+\mathcal{E}_{F,\varsigma}(\mathcal{M})\chi_{[0,1]}\subset L^1$ which has been estimated in Proposition 5.3.

5.5. Corollary. *Proposition 5.3 implies L^∞–estimates for the particle density operator. Thus, in connection with (2.9), one obtains L^p–bounds for the values of $\mathcal{N}_\varsigma$, $\varsigma\in\{1,\dots,\sigma\}$:*

$$\sup_{V\in\mathcal{M}}\left\|\mathcal{N}_\varsigma(V)\right\|_{L^p}\;\le\;N_\varsigma^{\frac1p}\sup_{V\in\mathcal{M}}\left\|\mathcal{N}_\varsigma(V)\right\|_{L^\infty}^{\frac{p-1}{p}}\;\le\;N_\varsigma^{\frac1p}\|\mathbb{1}\|^{\frac{p-1}{p}}_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\sup_{V\in\mathcal{M}}\left\|\mathcal{N}_\varsigma(V)\right\|^{\frac{p-1}{p}}_{W^{1,2}_\Gamma}$$

5.b. **Boundary behaviour.** In the next proposition we will deal with the boundary behaviour of the values of the pseudo particle density operator $\widetilde{\mathcal{N}}$, which naturally implies the same behaviour of the values of the operators $\mathcal{N}_\varsigma$. It is easy to prove that the particle densities vanish on the Dirichlet boundary part Γ, as the wave functions ψ_l do so there. Moreover, the derivative of $\widetilde{\mathcal{N}}(V)$ vanishes on the whole boundary of $\Omega=(0,1)$. In order to give an adequate formulation of this boundary behaviour, we prove the following

5.6. Lemma. *Let a potential $V\in L^1$ be given and let $\{\psi_l\}_l$ denote the system of (orthonormalized) eigenfunctions of the Schrödinger operator H_V, $\mathcal{E}_l$ the corresponding eigenvalues and $\mathcal{E}_F(V)$ the Fermi level. For every l the function $\psi_l\frac{1}{m}\psi_l'$ is continuous over $\overline{\Omega}=[0,1]$ and its values at the interval ends are zero. If f is a distribution function in accordance with Assumption 2.7, then the series*

$$\sum_{l=1}^{\infty} f(\mathcal{E}_l)\,\psi_l\,\frac{1}{m}\,\psi_l' \tag{5.8}$$

converges absolutely in C.

Proof. According to (3.17) and (3.9) there is

$$
(5.9)\quad \begin{aligned} \|\psi_l\|_{L^\infty} &\le \|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^\infty)} \overline{m}^{\frac{1}{2}} \left\|(H_0+1)^{\frac{1}{2}}\psi_l\right\| \\ &\le \|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^\infty)} \sqrt{2\,\overline{m}}\, \left\|(H_V-\rho)^{\frac{1}{2}}\psi_l\right\| \le \|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^\infty)} \sqrt{2\,\overline{m}\,(\mathcal{E}_l-\rho)}. \end{aligned}
$$

By Definition 2.3 of the operator H_V one has

$$
(5.10)\qquad \left(\frac{1}{m}\psi_l'\right)' = -V\psi_l + \mathcal{E}_l\,\psi_l \qquad \text{in the sense of distributions.}
$$

Because we already know that ψ_l is from L^∞, it is evident that the right hand side of (5.10) is from L^1 and one can estimate its L^1–norm:

$$
(5.11)\quad \begin{aligned} &\left\| -V\psi_l + \mathcal{E}_l\,\psi_l\right\|_{L^1} \\ &\quad\le \|V\|_{L^1}\,\|\psi_l\|_{L^\infty} + |\mathcal{E}_l|\,\|\psi_l\|_{L^1} \le \|V\|_{L^1}\,\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^\infty)} \sqrt{2\,\overline{m}\,(\mathcal{E}_l-\rho)} + |\mathcal{E}_l|. \end{aligned}
$$

Hence, the function $\frac{1}{m}\psi_l'$ is absolutely continuous and in particular continuous on $[0,1]$. We will now estimate its L^1–norm. First we rewrite the eigenvalue equation as

$$
\psi_l = (H_0+1)^{-1}\big(-V\psi_l + (\mathcal{E}_l+1)\psi_l\big),
$$

and estimate

$$
\begin{aligned} \|\psi_l\|_{W_\Gamma^{1,2}} &\le \left\|(H_0+1)^{-1}\right\|_{\mathcal{B}(W_\Gamma^{-1,2},W_\Gamma^{1,2})} \left\| -V\psi_l + (\mathcal{E}_l+1)\psi_l\right\|_{W_\Gamma^{-1,2}} \\ &\le \overline{m}\,\|\mathbb{1}\|_{\mathcal{B}(L^1,W_\Gamma^{-1,2})} \left\| -V\psi_l + (\mathcal{E}_l+1)\psi_l\right\|_{L^1} \\ &\le \overline{m}\,\|\mathbb{1}\|_{\mathcal{B}(L^1,W_\Gamma^{-1,2})} \left(\|V\|_{L^1}\,\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^\infty)} \sqrt{2\,\overline{m}\,(\mathcal{E}_l-\rho)} + |\mathcal{E}_l+1|\right). \end{aligned}
$$

Combining this with the trivial inequality

$$
\left\|\frac{1}{m}\psi_l'\right\|_{L^1} \le \left\|\frac{1}{m}\right\|_{L^\infty} \|\psi_l'\|_{L^2} \le \left\|\frac{1}{m}\right\|_{L^\infty} \|\psi_l\|_{W_\Gamma^{1,2}}
$$

one obtains the estimate

$$
(5.12)\quad \begin{aligned} &\left\|\frac{1}{m}\psi_l'\right\|_{L^1} \\ &\quad\le \left\|\frac{1}{m}\right\|_{L^\infty} \overline{m}\,\|\mathbb{1}\|_{\mathcal{B}(L^1,W_\Gamma^{-1,2})} \left(\|V\|_{L^1}\,\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^\infty)} \sqrt{2\,\overline{m}\,(\mathcal{E}_l-\rho)} + |\mathcal{E}_l+1|\right). \end{aligned}
$$

Next we estimate the supremum norm of $\frac{1}{m}\psi_l'$. If $x_0 \in [0,1]$ is a point, where $\frac{1}{m}|\psi_l'(\cdot)|$ takes its maximum, then

$$
(5.13)\quad \begin{aligned} \sup_{x\in[0,1]} \left|\frac{1}{m(x)}\psi_l'(x)\right| &= \left|\frac{1}{m(x_0)}\psi_l'(x_0)\right| = \int_0^1 \left|\frac{1}{m(x_0)}\psi_l'(x_0)\right| dx \\ &\le \int_0^1 \left|\frac{1}{m(x_0)}\psi_l'(x_0) - \frac{1}{m(x)}\psi_l'(x)\right| dx + \left\|\frac{1}{m}\psi_l'\right\|_{L^1}. \end{aligned}
$$

From (5.10) follows that the integrand on the right hand side of (5.13) is not greater than the L^1–norm of $-V\psi_l + \mathcal{E}_l\psi_l$. Thus, combining (5.13), (5.11) and (5.12) one obtains an upper bound for the supremum norm of $\frac{1}{m}\psi_l'$.

Both boundary points, $x = 0$ and $x = 1$, are either (homogeneous) Dirichlet ($\psi_l(x) = 0$) or Neumann boundary points. For the latter ones follows from the Definition 2.3 of H_0 by partial integration that $\frac{1}{m}\psi_l'(x) = 0$.

The uniform convergence of the series (5.8) follows from (5.10), (5.11), (5.12), (5.13), the asymptotical distribution of the eigenvalues $\mathcal{E}_l$, and the decay properties of the distribution functions f, cf. Assumption 2.7. □

5.7. Proposition. *For any $V \in L^1$ the particle density $\widetilde{\mathcal{N}}(V)$ (cf. Definition 2.9) has the following trace properties on the boundary of the domain $\Omega = (0,1)$:*

$$\widetilde{\mathcal{N}}(V)(x) = 0 \qquad \text{if } x \in \Gamma, \tag{5.14}$$

$$\frac{1}{m(x)} \frac{d\widetilde{\mathcal{N}}(V)}{dx}(x) = 0 \qquad \text{if } x \in \{0,1\}. \tag{5.15}$$

Proof. From (5.9) and the decay properties of the distribution functions f, cf. Assumption 2.7 immediately follows that the series (2.7) defining $\widetilde{\mathcal{N}}(V)$, converges in the space C. Hence, the property $\psi_l|_\Gamma = 0$ of the eigenfunctions carries over to the density $\widetilde{\mathcal{N}}(V)$. (5.15) directly follows from Lemma 5.6. □

5.8. Remark. If the effective mass function m is continuous in the boundary points 0 and 1, then (5.15) may be equivalently formulated as

$$\frac{d\widetilde{\mathcal{N}}(V)}{dx}(x) = 0 \qquad \text{if } x \in \{0,1\}.$$

5.c. Monotonicity.

5.9. Theorem. *We refer to the notation of Definition 2.9. For any $\varsigma \in \{1, \ldots, \sigma\}$ the negative particle density operator $-\mathcal{N}_\varsigma$ is a monotone operator from L^1 into L^∞ and a strictly monotone operator from $W^{1,2}_\Gamma$ into $W^{-1,2}_\Gamma$.*

The proof of these monotonicity properties is similar to that given in [6, 23, 25, 1]. It is based on the Fréchet differentiability of the particle density operator $\mathcal{N}_\varsigma$ and explicit calculation of

$$\Big\langle [\mathcal{N}_\varsigma'(V)]\, W \,,\, W \Big\rangle \qquad \text{for all} \quad W \in L^\infty, \quad V \in W^{1,2}_\Gamma.$$

The resulting expression turns out positive due to the monotonicity properties of the distribution function f_ς, cf. Assumption 2.7.

6. Existence of solutions and a priori estimates

In this section we present our central results. We recall the convention from §2 that symbols with a hat refer to the spatial domain $\widehat{\Omega} = (a,b)$, while the symbols without a hat are reserved for spaces which refer to the spatial domain $\Omega = (0,1)$, cf. Remark 2.2.

6.a. The linear Poisson operator.

6.1. Lemma. *The operator $A : \widehat{W^{1,2}_{\widehat{\Gamma}}} \mapsto \widehat{W^{-1,2}_{\widehat{\Gamma}}}$ from Definition 2.13 is strongly monotone and Lipschitz continuous.*

$$\frac{1}{m_A} = c_k \max\left\{1, \left\|\varepsilon^{-1}\right\|_{\widehat{L^\infty}}\right\} \tag{6.1}$$

serves as a monotonicity constant and

$$M_A = \|\varepsilon\|_{L^\infty(\hat{\Omega})} + \|\mathbb{1}\|^2_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}}, \widehat{C})} \sum_{x \in \{a,b\} \setminus \widehat{\Gamma}} k(x) \tag{6.2}$$

as a Lipschitz constant, where $\|\mathbb{1}\|_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}}, \widehat{C})}$ denotes the embedding constant from $\widehat{W^{1,2}_{\widehat{\Gamma}}}$ into $\widehat{C}$, which is finite in one dimension.

Proof. First we observe

$$\|u'\|^2_{\widehat{L^2}} = \left\|\varepsilon^{-\frac{1}{2}}\varepsilon^{\frac{1}{2}}u'\right\|^2_{\widehat{L^2}} \le \|\varepsilon^{-1}\|_{\widehat{L^\infty}} \|\varepsilon^{\frac{1}{2}}u'\|^2_{\widehat{L^2}} = \|\varepsilon^{-1}\|_{\widehat{L^\infty}} \int_a^b \varepsilon(x)\big(u'(x)\big)^2\,dx.$$

Now one easily deduces from the definition of A and c_k, cf. Definition 2.13,

$$\begin{aligned}
\|u\|^2_{\widehat{W^{1,2}_{\Gamma}}} &\le c_k \Big(\|u'\|^2_{\widehat{L^2}} + \sum_{x\in\{a,b\}\setminus\widehat{\Gamma}} k(x)\big|u(x)\big|^2\Big)\\
&\le c_k\Big(\|\varepsilon^{-1}\|_{\widehat{L^\infty}} \int_a^b \varepsilon(x)\,u'(x)\,u'(x)\,dx + \sum_{x\in\{a,b\}\setminus\widehat{\Gamma}} k(x)\big|u(x)\big|^2\Big)\\
&\le c_k \max\big\{1, \|\varepsilon^{-1}\|_{\widehat{L^\infty}}\big\}\,\big\langle Au, u\big\rangle.
\end{aligned}$$

N.B. k is nonnegative. To prove the second assertion, we estimate the norm of A

$$M_A = \|A\|_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},\widehat{W^{-1,2}_{\widehat{\Gamma}}})} = \sup_{\|u\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}=\|v\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}=1} \big|\langle Au, v\rangle\big|$$

by means of

$$\begin{aligned}
\big|\langle Au, v\rangle\big| &= \Big|\int_a^b \varepsilon(x)\,u'(x)\,v'(x)\,dx + \sum_{x\in\{a,b\}\setminus\widehat{\Gamma}} k(x)\,u(x)\,v(x)\Big|\\
&\le \left(\|\varepsilon\|_{\widehat{L^\infty}} + \sum_{x\in\{a,b\}\setminus\widehat{\Gamma}} k(x)\,\|\mathbb{1}\|^2_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},\widehat{C})}\right)\|u\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}\|v\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}.
\end{aligned}$$

□

6.b. **The nonlinear Schrödinger–Poisson operator.** Up to now we have regarded the particle density operators as operators from L^1 into function spaces over $\Omega = (0,1)$. From now on we will regard the system as a whole and therefore consider the particle density operators as operators with values in suitable function spaces over $\widehat{\Omega} = (a,b)$ by means of the identification operators Z^*_ς from Definition 2.14. In the following $\mathbf{V} = (V_1,\dots,V_\sigma) \in (L^1)^\sigma$ is a given σ–tuple of external potentials.

The statements of the next proposition follow directly from Theorem 5.9 and the Lipschitz properties of the operators $\mathcal{N}_\varsigma$ (cf. §5.a).

6.2. Proposition. *For any $\varsigma \in \{1,\dots,\sigma\}$ the negative extended particle density operator*

$$\widehat{W^{1,2}_{\widehat{\Gamma}}} \ni V \longmapsto -Z^*_\varsigma \mathcal{N}_\varsigma\big(V_\varsigma + Z_\varsigma V\big) \in \widehat{W^{-1,2}_{\widehat{\Gamma}}}$$

is monotone. Moreover, this operator is locally Lipschitz continuous, and its local Lipschitz constant on a bounded set $\widehat{\mathcal{M}} \subset \widehat{W^{1,2}_{\widehat{\Gamma}}}$ is not greater than

$$\|Z_\varsigma\|^2_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},L^1)}\,\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\,\mathbf{Lip}_{(V_\varsigma+Z_\varsigma\widehat{\mathcal{M}})}(\mathcal{N}_\varsigma), \tag{6.3}$$

where $\mathbf{Lip}_{(V_\varsigma+Z_\varsigma\widehat{\mathcal{M}})}(\mathcal{N}_\varsigma)$ is the local Lipschitz constant of the mapping $\mathcal{N}_\varsigma : L^1 \longmapsto W^{1,2}_\Gamma$, restricted to the set $V_\varsigma + Z_\varsigma\widehat{\mathcal{M}}$, cf. Corollary 5.4.

Proposition 6.2 implies by means of Theorem 2.17 the following

6.3. Proposition. *The nonlinear Schrödinger–Poisson operator*

$$P_{\mathbf{V}} : \widehat{W^{1,2}_{\widehat{\Gamma}}} \mapsto \widehat{W^{-1,2}_{\widehat{\Gamma}}}, \quad P_{\mathbf{V}} V = AV - \sum_{\varsigma\in\{1,\dots,\sigma\}} Z_\varsigma^* \mathcal{N}_\varsigma\big(V_\varsigma + Z_\varsigma V\big) - F_\varsigma(V) \tag{6.4}$$

is strongly monotone with m_A *as a monotonicity constant. Additionally, this operator is locally Lipschitz continuous. More precisely, if* $\widehat{\mathcal{M}}$ *is a bounded set in* $\widehat{W^{1,2}_{\widehat{\Gamma}}}$*, then the local Lipschitz constant of* $P_{\mathbf{V}}$*, corresponding to the set* $\widehat{\mathcal{M}}$ *is*

$$\begin{aligned}\mathbf{Lip}_{\widehat{\mathcal{M}}}(P_{\mathbf{V}}) \le M_A &+ \sum_{\varsigma\in\{1,\dots,\sigma\}} \mathbf{Lip}_{\widehat{\mathcal{M}}}(F_\varsigma) \\ &+ \sum_{\varsigma\in\{1,\dots,\sigma\}} \|Z_\varsigma\|^2_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},L^1)} \|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\Gamma},L^\infty)} \mathbf{Lip}_{(V_\varsigma+Z_\varsigma\widehat{\mathcal{M}})}(\mathcal{N}_\varsigma),\end{aligned} \tag{6.5}$$

where $\mathbf{Lip}_{\widehat{\mathcal{M}}}(F_\varsigma)$ *is the local Lipschitz constant of the mapping* F_ς *defined in Assumption 2.6. The nonlinear Poisson equation*

$$P_{\mathbf{V}} V = D \tag{6.6}$$

admits exactly one solution $\underline{V}$ *for every effective doping profile* $D \in \widehat{W^{-1,2}_{\widehat{\Gamma}}}$ *(cf. Definition 2.14). This solution satisfies the estimate*

$$\|\underline{V}\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} \le \frac{1}{m_A}\Big\|D + \sum_{\varsigma\in\{1,\dots,\sigma\}} Z_\varsigma^*\mathcal{N}_\varsigma(V_\varsigma) + F_\varsigma(0)\Big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}. \tag{6.7}$$

If $\mathcal{J} : \widehat{W^{1,2}_{\widehat{\Gamma}}} \longmapsto \widehat{W^{-1,2}_{\widehat{\Gamma}}}$ *is the duality mapping and* M_P *the local Lipschitz constant* (6.5) *of the mapping* $P_{\mathbf{V}}$ *which corresponds to a centered ball in* $\widehat{W^{1,2}_{\widehat{\Gamma}}}$ *with radius not smaller than*

$$\frac{2}{m_A}\Big\|D + \sum_{\varsigma\in\{1,\dots,\sigma\}} Z_\varsigma^*\mathcal{N}_\varsigma(V_\varsigma) + F_\varsigma(0)\Big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}, \tag{6.8}$$

then the solution $\underline{V}$ *of* (6.6) *is obtained as the fixed point of the mapping*

$$Q_{\mathbf{V}} : \widehat{\mathcal{M}} \longmapsto \widehat{\mathcal{M}}, \qquad Q_{\mathbf{V}} : V \longmapsto V - \frac{m_A}{M_P^2}\mathcal{J}^{-1}\big(P_{\mathbf{V}}V - D\big), \tag{6.9}$$

which is contractive on $\widehat{\mathcal{M}}$ *with the contraction constant*

$$\sqrt{1 - \frac{m_A^2}{M_P^2}}. \tag{6.10}$$

6.4. Remark. In the standard case, where the operator Z_ς^* is the extension operator by zero on $[a,b] \setminus [0,1]$ (cf. Remark 2.15), the a priori estimate (6.7) may be expressed in terms of the total charges N_ς:

$$\begin{aligned}\big\|Z_\varsigma^*\mathcal{N}_\varsigma(V_\varsigma)\big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}} &\le \|\mathbb{1}\|_{\mathcal{B}(\widehat{L^1},\widehat{W^{-1,2}_{\widehat{\Gamma}}})} \big\|Z_\varsigma^*\mathcal{N}_\varsigma(V_\varsigma)\big\|_{\widehat{L^1}} \\ &= \|\mathbb{1}\|_{\mathcal{B}(\widehat{L^1},\widehat{W^{-1,2}_{\widehat{\Gamma}}})} \big\|\mathcal{N}_\varsigma(V_\varsigma)\big\|_{L^1} = \|\mathbb{1}\|_{\mathcal{B}(\widehat{L^1},\widehat{W^{-1,2}_{\widehat{\Gamma}}})} N_\varsigma.\end{aligned} \tag{6.11}$$

From Proposition 6.3 one easily deduces

6.5. Theorem. *The Schrödinger–Poisson system without exchange–correlation potential (cf. Definition 2.14) has the unique solution* $\big(\underline{V}, \widetilde{\mathcal{N}}_1(V_1+\underline{V}), \dots, \widetilde{\mathcal{N}}_\sigma(V_\sigma+\underline{V})\big)$*, where* $\underline{V}$ *is the fixed point of the operator* (6.9).

6.6. Remark. It is not difficult to see that the main content of this subsection remains true if the operator Z^* is replaced by an operator lying in a suitable neighbourhood of Z^*. In particular, the operator $P_{\mathbf{V}}$, constructed this way, satisfies similar monotonicity and Lipschitz properties, and the theory of monotone operators still applies.

Next we will have a look on the dependence of the solution of the nonlinear Schrödinger–Poisson equation (6.6) on the vector $\mathbf{V} = (V_1, \dots, V_\sigma) \in (L^1)^\sigma$ of external potentials.

6.7. Lemma. *Let*

$$\mathcal{L} : (L^1)^\sigma \longmapsto \widehat{W^{1,2}_{\widehat{\Gamma}}}, \qquad \mathcal{L}(\mathbf{V}) = \underline{V} \tag{6.12}$$

be the operator, which assigns to the σ–tuple $\mathbf{V} = (V_1, \dots, V_\sigma) \in (L^1)^\sigma$ *of external potentials the solution* $\underline{V}$ *of the equation* (6.6)*. If* $\mathcal{M}$ *is a bounded set in* L^1*, then*

$$\sup_{\mathbf{V}\in\mathcal{M}^\sigma} \left\|\mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} \le \frac{1}{m_A}\Bigg(q\left\|N_A - N_D\right\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}} + \|\varepsilon\|_{\widehat{L^\infty}}\left\|\varphi_{\widehat{\Gamma}}\right\|_{\widehat{W^{1,2}}} + \sum_{\varsigma\in\{1,\dots,\sigma\}} \left(\left\|F_\varsigma(0)\right\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}} + \sup_{V\in\mathcal{M}} \left\|Z_\varsigma^*\mathcal{N}_\varsigma(V)\right\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}} \right)\Bigg). \tag{6.13}$$

The mapping $\mathcal{L}$ *is boundedly Lipschitz continuous from* $(L^1)^\sigma$ *into* $\widehat{W^{1,2}_{\widehat{\Gamma}}}$*, and its local Lipschitz constant corresponding to* $\mathcal{M}^\sigma$ *is not greater than*

$$\frac{2}{m_A}\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\Gamma},L^\infty)} \sup_{\varsigma\in\{1,\dots,\sigma\}} \|Z_\varsigma\|_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},L^1)} \sum_{\varsigma\in\{1,\dots,\sigma\}} \mathbf{Lip}_{(\mathcal{M}+Z_\varsigma\mathcal{L}(\mathcal{M}^\sigma))}(\mathcal{N}_\varsigma), \tag{6.14}$$

where $\mathbf{Lip}_{(\mathcal{M}+Z_\varsigma\mathcal{L}(\mathcal{M}^\sigma))}(\mathcal{N}_\varsigma)$ *is the local Lipschitz constant of the mapping* $\mathcal{N}_\varsigma : L^1 \mapsto W^{1,2}_\Gamma$*, cf. Corollary 5.4, restricted to the set* $\mathcal{M} + Z_\varsigma\mathcal{L}(\mathcal{M}^\sigma)$*.*

Proof. By definition of $\mathcal{L}$, $\underline{V} = \mathcal{L}(\mathbf{V})$ is a solution of (6.6) and, hence, satisfies the estimate (6.7). Taking into account (2.15), and the inequality

$$\left\|\widetilde{\varphi}_{\widehat{\Gamma}}\right\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}} \le \|\varepsilon\|_{\widehat{L^\infty}}\left\|\varphi_{\widehat{\Gamma}}\right\|_{\widehat{W^{1,2}}}$$

this implies the first assertion.

For the proof of the local Lipschitz continuity, let $\mathbf{U} = (U_1, \dots, U_\sigma)$ and $\mathbf{V} = (V_1, \dots, V_\sigma)$ from $\mathcal{M}^\sigma$ be given. $\mathcal{L}(\mathbf{V})$ is the fixed point of the strict contraction $Q_{\mathbf{V}}$ defined in (6.9), and $\mathcal{L}(\mathbf{U})$ is the fixed point of $Q_{\mathbf{U}}$. Hence,

$$\begin{aligned} \left\|\mathcal{L}(\mathbf{U}) - \mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} &= \left\|Q_{\mathbf{U}}\mathcal{L}(\mathbf{U}) - Q_{\mathbf{V}}\mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} \\ &\le \left\|Q_{\mathbf{U}}\mathcal{L}(\mathbf{U}) - Q_{\mathbf{U}}\mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} + \left\|(Q_{\mathbf{U}} - Q_{\mathbf{V}})\mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}. \end{aligned}$$

Taking into account the Lipschitz constant (6.10) of $Q_{\mathbf{U}}$, one easily deduces

$$\left\|\mathcal{L}(\mathbf{U}) - \mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} \le \left(1 - \sqrt{1 - \frac{m_A^2}{M_P^2}}\right)^{-1} \left\|(Q_{\mathbf{U}} - Q_{\mathbf{V}})\mathcal{L}(\mathbf{V})\right\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}.$$

Now using the definition of $Q_{\mathbf{U}}$ and $Q_{\mathbf{V}}$ and the inequality

$$\frac{\frac{m_A}{M_P^2}}{1 - \sqrt{1 - \frac{m_A^2}{M_P^2}}} \le \frac{2}{m_A}$$

one arrives at

$$
\begin{aligned}
&\big\|\mathcal{L}(\mathbf{U})-\mathcal{L}(\mathbf{V})\big\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}}\\
&\le \frac{2}{m_A}\Big\|\mathcal{J}^{-1}\big(P_{\mathbf{U}}-P_{\mathbf{V}}\big)\mathcal{L}(\mathbf{V})\Big\|_{\widehat{W^{1,2}_{\widehat{\Gamma}}}} \le \frac{2}{m_A}\Big\|\big(P_{\mathbf{U}}-P_{\mathbf{V}}\big)\mathcal{L}(\mathbf{V})\Big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}\\
&\le \frac{2}{m_A}\Big\|\sum_{\varsigma\in\{1,\dots,\sigma\}} Z_\varsigma^*\mathcal{N}_\varsigma\big(U_\varsigma+Z_\varsigma\mathcal{L}(\mathbf{V})\big)-Z_\varsigma^*\mathcal{N}_\varsigma\big(V_\varsigma+Z_\varsigma\mathcal{L}(\mathbf{V})\big)\Big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}\\
&\le \frac{2}{m_A}\sup_{\varsigma\in\{1,\dots,\sigma\}}\|Z_\varsigma\|_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},L^1)}\Big\|\sum_{\varsigma\in\{1,\dots,\sigma\}}\mathcal{N}_\varsigma\big(U_\varsigma+Z_\varsigma\mathcal{L}(\mathbf{V})\big)-\mathcal{N}_\varsigma\big(V_\varsigma+Z_\varsigma\mathcal{L}(\mathbf{V})\big)\Big\|_{L^\infty},
\end{aligned}
$$

and finally at the Lipschitz constant (6.14). □

6.c. **The Kohn–Sham system.** We will now introduce an adequate subset of $(L^1)^\sigma$ and a suitable mapping Φ from this set into itself the fixed points of which will provide solutions for the Kohn–Sham system i.e. the Schrödinger–Poisson system with an exchange–correlation potential.

6.8. Definition. Let $\mathbf{V}=(V_1,\dots,V_\sigma)\in(L^1)^\sigma$ be a given σ–tuple of external potentials and $N_1,\dots,N_\sigma$, the fixed numbers of carriers, cf. Definition 2.9. We define

$$
L^1_N=\Big\{\mathbf{u}=(u_1,\dots,u_\sigma): u_\varsigma\ge 0,\ \int_0^1 u_\varsigma(x)dx=N_\varsigma,\ \varsigma\in\{1,\dots,\sigma\}\Big\} \tag{6.15}
$$

and $\Phi: L^1_N\longmapsto L^1_N$ as the mapping whose ς–component is given by

$$
\Phi_\varsigma(\mathbf{u})=\mathcal{N}_\varsigma\Big(V_\varsigma+V_{xc,\varsigma}(\mathbf{u})+Z_\varsigma\mathcal{L}\big(V_1+V_{xc,1}(\mathbf{u}),\dots,V_\sigma+V_{xc,\sigma}(\mathbf{u})\big)\Big). \tag{6.16}
$$

6.9. Lemma. *For any $\varsigma\in\{1,\dots,\sigma\}$ let $V_{xc,\varsigma}$ be a bounded and continuous mapping from $(L^1)^\sigma$ into L^1. If*

$$
\delta=\sup_{\varsigma\in\{1,\dots,\sigma\}}\ \sup_{\mathbf{u}\in L^1_N}\big\|V_{xc,\varsigma}(\mathbf{u})\big\|_{L^1} \tag{6.17}
$$

and

$$
\mathcal{M}=\Big\{V\in L^1:\ \max_{\varsigma\in\{1,\dots,\sigma\}}\|V-V_\varsigma\|_{L^1}\le\delta\Big\}, \tag{6.18}
$$

then the number

$$
\begin{aligned}
s=\sup_{\varsigma\in\{1,\dots,\sigma\}}\|V_\varsigma\|_{L^1}+\delta+\frac{1}{m_A}\Big(\sup_{\varsigma\in\{1,\dots,\sigma\}}\|Z_\varsigma\|_{\mathcal{B}(\widehat{W^{1,2}_{\widehat{\Gamma}}},L^1)}\Big)\Bigg(q\,\|N_A-N_D\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}\\
+\|\varepsilon\|_{\widehat{L^\infty}}\,\|\varphi_{\widehat{\Gamma}}\|_{\widehat{W^{1,2}}}+\sum_{\varsigma\in\{1,\dots,\sigma\}}\Big(\big\|F_\varsigma(0)\big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}+\sup_{V\in\mathcal{M}}\big\|Z_\varsigma^*\mathcal{N}_\varsigma(V)\big\|_{\widehat{W^{-1,2}_{\widehat{\Gamma}}}}\Big)\Bigg)
\end{aligned} \tag{6.19}
$$

is a common upper bound for the L^1–norm of the Schrödinger potentials which are involved in the definition of the carrier densities in (6.16)*, and*

$$
\rho=-\frac{1}{2}\gamma_1^4\max_{\varsigma\in\{1,\dots,\sigma\}}\max\left(1,\frac{2\,\|m_\varsigma\|_{L^\infty}}{\hbar^2}\right)s^2-1 \tag{6.20}
$$

is the corresponding quantity (3.13)*. Any element from the range of Φ does not only belong to L^1_N, but satisfies the a priori estimates given in Proposition 5.3, where the s–ball in L^1 serves as the set $\mathcal{M}$ in §5.a.*

Proof. For the proof it suffices to show that s is an L^1–bound for the sets

$$V_\varsigma + V_{xc,\varsigma}(L^1_N) + Z_\varsigma \mathcal{L}\big(V_1 + V_{xc,1}(L^1_N), \dots, V_\sigma + V_{xc,\sigma}(L^1_N)\big), \qquad \varsigma \in \{1, \dots, \sigma\}$$

and then to apply Proposition 5.3. (6.17) implies

$$\big\| V_{xc,\varsigma}(\mathbf{u}) \big\|_{L^2} \le \delta \qquad \text{for all } \mathbf{u} \in L^1_N, \qquad \varsigma \in \{1, \dots, \sigma\}.$$

The right hand side of (6.13) provides a $\widehat{W^{1,2}_{\Gamma}}$–bound for all

$$\mathcal{L}\big(V_1 + V_{xc,1}(\mathbf{u}), \dots, V_\sigma + V_{xc,\sigma}(\mathbf{u})\big), \qquad \text{with } \mathbf{u} \in L^1_N,$$

where $\mathcal{M}$ is defined by (6.18). From this, the required L^1-bound of $Z_\varsigma \mathcal{L}(\dots)$ is easily deduced. □

6.10. Remark. Often the exchange–correlation terms $V_{xc,\varsigma}$ are given by rational expressions as e.g. (1.9) which allow to estimate the quantity δ in Lemma 6.9 in terms of the data of the problem. If $\alpha_\varsigma \le 1$ (as supposed in (1.9)), then

$$\delta \le \sup_{\varsigma \in \{1, \dots, \sigma\}} \beta_\varsigma N_\varsigma^{\alpha_\varsigma}. \tag{6.21}$$

Now we are ready to prove the existence theorem for the Schrödinger–Poisson system with an exchange–correlation potential.

6.11. Theorem. *If $V_{xc,\varsigma}$ is for any $\varsigma \in \{1, \dots, \sigma\}$ a bounded and continuous mapping from $(L^1)^\sigma$ into L^1, then the mapping Φ from Definition 6.8 has a fixed point.*

Proof. It is evident that Φ maps L^1_N into itself (cf. Definition 6.8 and Definition 2.9). From the continuity properties of the mappings $V_{xc,\varsigma}$, $\mathcal{N}_\varsigma$, and $\mathcal{L}$ (cf. §5.a and Lemma 6.7) directly follows that Φ is continuous. Lemma 6.9 assures that the image of Φ is bounded in the space $\big(W^{1,2}_\Gamma\big)^\sigma$, hence, it is precompact in $(L^1)^\sigma$. Thus, according to Schauder's fixed point theorem, Φ has a fixed point in L^1_N. □

6.12. Remark. The fixed point mapping used in this proof was proposed by Herbert Gajewski in the seminar of Arno Langenbach.

6.13. Corollary. *The particle densities u_ς of a fixed point $\mathbf{u} = (u_1, \dots, u_\sigma)$ of Φ do not only belong to L^1, but satisfy the estimates given in Proposition 5.3, where ρ is defined by (6.20).*

Proof. Obviously any fixed point is contained in the image of Φ and, hence, obeys the a priori estimates stated in Lemma 6.9. □

6.14. Theorem. $\mathbf{u} = (u_1, \dots, u_\sigma)$ *is a fixed point of Φ if and only if*

$$(V, u_1, \dots, u_\sigma) = \Big(A^{-1}\Big(D + \sum_{\varsigma \in \{1, \dots, \sigma\}} Z^*_\varsigma u_\varsigma\Big), u_1, \dots, u_\sigma\Big) \tag{6.22}$$

is a solution of the Kohn-Sham system, cf. Definition 2.14. In particular, this means that the Kohn-Sham system always admits a solution.

Proof. It follows from Definition 6.8 and Definition 2.14 that any solution of the Kohn–Sham system is a fixed point of the mapping Φ. Any fixed point $\mathbf{u} = \Phi\mathbf{u}$ defines via (6.22) a solution of the Kohn–Sham system in the sense of Definition 2.14. This is a consequence of the definition (6.12) of $\mathcal{L}$ and Corollary 6.13. □

6.15. Remark. Obviously the (homogenized) electrostatic potential

$$V = A^{-1}\left(D + \sum_{\varsigma\in\{1,\dots,\sigma\}} Z_\varsigma^* u_\varsigma\right)$$

belongs to the space $\widehat{W_\Gamma^{1,2}}$. Reiterating this argument, one obtains in smooth situations — where the coefficients are smooth and the boundary conditions are not mixed — that the particle densities and the electrostatic potential of a solution are infinitely smooth.

6.16. Remark. Corollary 6.13 justifies to demand in Definition 2.14 that a solution of the Schrödinger–Poisson system has carrier densities u_ς from the space L^∞.

7. Uniqueness of solutions

In sharp contrast to the situation of a vanishing exchange–correlation term in the potential of Schrödinger's equation, no general results concerning uniqueness of solutions of the Kohn–Sham system are known to the authors. However, if the exchange–correlation terms do not change rapidly, then one can prove that the solution remains unique.

7.1. Remark. A specific difficulty is that the generic exchange–correlation potentials (1.9) are not Lipschitz continuous. However, the expressions (1.9) are not properly justified for very low carrier densities u_ς and the following regularization is possible [28]

$$V_{xc,\varsigma}(\mathbf{u}) = \beta_\varsigma\, \delta_\varsigma^{\alpha_\varsigma} - \beta_\varsigma\left(u_\varsigma + \delta_\varsigma\right)^{\alpha_\varsigma}, \quad \beta_\varsigma > 0, \quad 0 \le \alpha \le 1 \tag{7.1}$$

This mapping $V_{xc,\varsigma} : (L^1)^\sigma \longmapsto L^1$ is Lipschitz continuous.

7.2. Theorem. *If the mappings $V_{xc,\varsigma}$ are boundedly Lipschitz continuous from $(L^1)^\sigma$ into L^1 on the set L^1_N, and the corresponding Lipschitz constants are sufficiently small, then the solution of the Kohn–Sham system is unique (cf. Definition 2.14 and Definition 6.8).*

Proof. One again regards the mapping $\Phi : L^1_N \longmapsto L^1_N$ from Definition 6.8. Combining the results on Φ from §6.c and the Lipschitz properties of the mappings $V_{xc,\varsigma}$, $\mathcal{L}$ (cf. Lemma 6.7), Z_ς (cf. Definition 2.14), and $\mathcal{N}_\varsigma$ (cf. Corollary 5.4), one obtains that Φ is a Lipschitz continuous mapping from L^1_N into itself.

$$\mathbf{Lip}_{L^1_N}(\Phi_\varsigma) = \mathbf{Lip}_{\substack{s\text{-ball}\\ \text{in } L^1}}(\mathcal{N}_\varsigma)\left(1 + \|Z_\varsigma\|_{\mathcal{B}(\widehat{W_\Gamma^{1,2}},L^1)}\mathbf{Lip}_{\mathcal{M}^\sigma}(\mathcal{L})\right)\sup_{\varsigma\in\{1,\dots,\sigma\}}\mathbf{Lip}_{L^1_N}(V_{xc,\varsigma})$$

is a Lipschitz constant of the ς–component (6.16) of Φ, where $\mathcal{M}$ is the set (6.18), and s is the number (6.19). Thus, if the Lipschitz constants $\mathbf{Lip}_{L^1_N}(V_{xc,\varsigma})$ of the mappings $V_{xc,\varsigma}$, $\varsigma \in \{1,\dots,\sigma\}$ are sufficiently small, then Banach's fixed point principle provides a unique solution of the Kohn–Sham system. □

7.3. Remark. In the sense of Remark 6.10 one often can estimate the Lipschitz constant of $V_{xc,\varsigma}$ in terms of the data of the problem. The Lipschitz constants of $\mathcal{L}$ and $\mathcal{N}_\varsigma$ also can be estimated in terms of these data, cf. Lemma 6.7 and Corollary 5.4 respectively. Thus, in principle one can get ranges of data which assure uniqueness. N.B. for this purpose the Birman–Solomjak Theorem 2.19 is essential, as it puts the cutting edge to our estimates. It is not known yet, however, whether the uniqueness assuring ranges of data, which are determined that way, are pessimistic or really interesting from a physical point of view.

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