ABOUT A STATIONARY SCHRÖDINGER–POISSON SYSTEM WITH KOHN–SHAM POTENTIAL IN NANOELECTRONICS

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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.

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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 di-

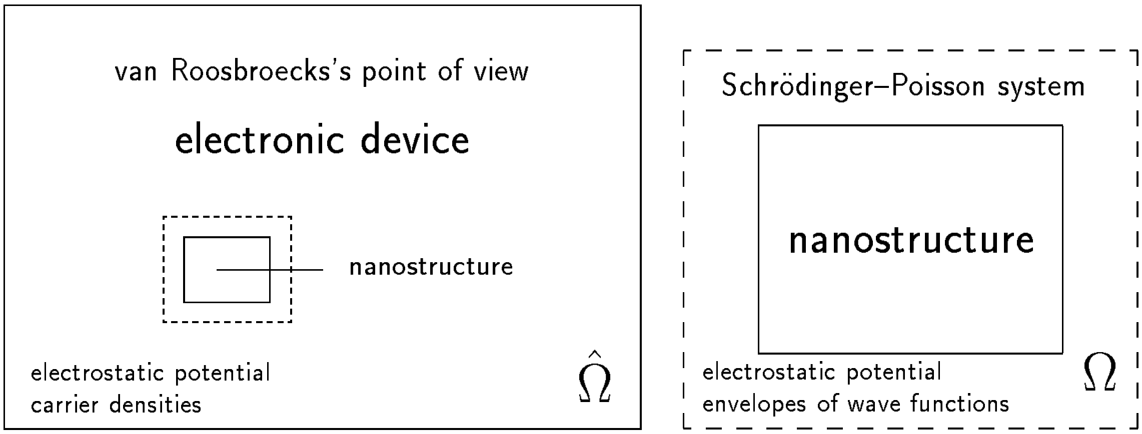

FIGURE 1. Around the nanostructure and beyond

rections 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. [46, 16, 29, 45, 17]). 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. [16, 17]). For a two–, one– or zero–dimensional carrier gas the dimension d of the (bounded) spatial domain $\Omega \subset \hat{\Omega} \subset \mathbb{R}^d$, where we regard the system, is $d = 1, 2, 3$, respectively.

The coupling of the nanostructure to its enviroment is a widely discussed task in modelling and simulation of semiconductor nanostructures (cf. e.g. [6, 4, 16, 29, 30, 31, 45, 46]), but it is open to mathematical validation [20]. 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 [17] for the electrostatic potential. In view of modelling equilibrium situations we regard Schrödinger's operator with mixed hard–wall and harmonic boundary conditions (1.18). 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.c. When leaving equilibrium situations, of course, in general there should be currents over the boundary of the nanostructure [16, 6]. Proper conditions at the interface of the nanostructure and its enviroment are:

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

Aiming at the inclusion of the Schrödinger–Poisson system into Van Roosbroeck's equations (cf. [25]) 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 (cf. [24]):

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

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.

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. [12, 35, 36, 17, 1, 27, 26]).

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. 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 [27, 26]. 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 [7, 8].

The analytical properties of the Schrödinger–Poisson system pass to the discretized system (cf. [12, 1]), thus allowing proper implementation of the above mentioned iterations, e.g. based on a finite box method as in [18].

Our calculus for the Schrödinger–Poisson system with certain exchange–correlation potentials is based upon the results for the system without exchange–correlation potential. First one can prove that the solution of the Schrödinger–Poisson system 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 $L^1(\Omega)$ on a potential from $L^2(\Omega)$. The physically relevant exchange–correlation potentials in the two– and three–dimensional case belong to that class. If the exchange–correlation potential is Lipschitz continuous and sufficiently small, then the solution of the Kohn–Sham system is unique. As the exchange–correlation potentials in general are only from L^2, we need a calculus for Schrödinger operators with potentials from L^2. In contrast to the quantum Vlasov equation (cf. [33]), this seems to be an appropriate setting for the Schrödinger–Poisson equations. Indeed, we get non–negative carrier densities from the space L^1, in fact, they are even much more regular. Our present approach to the Kohn–Sham system rests upon the supposed L^1–norm conservation for each kind of carriers, cf. also Remark 6.16. 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 (cf. Appendix A.2). 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 Kohn–Sham system

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

$$(1.1) \qquad -\operatorname{div}\big(\varepsilon \operatorname{grad}\varphi\big) = q\Big(N_A - N_D + \sum_{\varsigma\in\{1,\dots,\sigma\}} e_\varsigma u_\varsigma\Big) \quad \text{in } \hat{\Omega}$$

in the device domain $\hat{\Omega}$. 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 tensor. 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 (1.6). Outside the nanostructure there are the state equations

$$(1.2) \qquad u_\varsigma(x) = \mathcal{F}_\varsigma\Big(-e_\varsigma\big(\varphi(x) - \phi_\varsigma(x)\big)\Big) \quad x \in \hat{\Omega}\setminus\Omega,$$

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. [17]), i.e.

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

where $\mathfrak{F}_\alpha(\zeta)$ denotes Fermi's integral ($\alpha > -1$) and Fermi's function ($\alpha = -1$) respectively:

$$(1.4) \qquad \mathfrak{F}_\alpha(\zeta) = \begin{cases} \frac{1}{\Gamma(\alpha+1)}\int_0^\infty \frac{\xi^\alpha}{1+\exp(\xi-\zeta)}d\xi & \text{if } \alpha > -1 \\ \frac{1}{1+\exp(-\zeta)} & \text{if } \alpha = -1 \end{cases} \qquad \zeta\in\mathbb{R}$$

$$(1.5) \qquad \mathfrak{F}'_\alpha(\zeta) = \mathfrak{F}_{\alpha-1}(\zeta), \qquad \alpha \geq 0, \qquad \zeta\in\mathbb{R}.$$

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

$$(1.6) \qquad u_\varsigma(\mathfrak{V}_\varsigma)(x) = \sum_{l=1}^{\infty} N_{l,\varsigma}(\mathfrak{V}_\varsigma)\left|\psi_{l,\varsigma}(\mathfrak{V}_\varsigma)(x)\right|^2, \quad x\in\Omega, \quad \varsigma\in\{1,\dots,\sigma\}.$$

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

$$(1.7) \qquad N_{l,\varsigma}(\mathfrak{V}_\varsigma) = f_\varsigma\left(\mathcal{E}_{l,\varsigma}(\mathfrak{V}_\varsigma) - \mathcal{E}_{F,\varsigma}(\mathfrak{V}_\varsigma)\right), \quad \varsigma\in\{1,\dots,\sigma\},$$

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 $\mathfrak{V}_\varsigma$

$$\left[-\frac{\hbar^2}{2}\operatorname{div}\left(m_\varsigma^{-1}\operatorname{grad}\right) + \mathfrak{V}_\varsigma\right]\psi_{l,\varsigma} = \mathcal{E}_{l,\varsigma}\psi_{l,\varsigma} \quad \text{in } \Omega, \tag{1.8}$$

where $m_\varsigma = m_\varsigma(x)$ is the Ω–component of the position dependent effective–mass tensor of ς–type carriers.

The effective Kohn–Sham potentials depend on the carrier densities, and split up in the following way

$$\mathfrak{V}_\varsigma(\mathbf{u}) = -e_\varsigma \Delta E_\varsigma + V_{xc,\varsigma}(\mathbf{u}) + e_\varsigma q \varphi(\mathbf{u})|_\Omega, \tag{1.9}$$

where $\varphi(\mathbf{u})|_\Omega$, denotes the restriction of the electrostatic potential $\varphi(\mathbf{u})$ to the domain Ω of the nanostructure, cf. (1.1). 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

$$V_{xc,\varsigma}(\mathbf{u}) = -\beta_\varsigma u_\varsigma^\alpha, \qquad \beta_\varsigma > 0, \quad \varsigma \in \{1,\dots,\sigma\} \tag{1.10}$$

where $\alpha = \frac{1}{d}$ for $d = 2,3$ (cf. Appendix A.1).

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

$$N_\varsigma = \int_\Omega u_\varsigma(\mathfrak{V}_\varsigma)(x)dx = \sum_{l=1}^\infty f_\varsigma(\mathcal{E}_{l,\varsigma}(\mathfrak{V}_\varsigma) - \mathcal{E}_{F,\varsigma}(\mathfrak{V}_\varsigma)), \tag{1.11}$$

N_ς being the fixed total number of ς–type carriers in the nanostructure domain Ω under consideration.

The distribution functions $f = f_\varsigma$, $\varsigma \in \{1,\dots,\sigma\}$ take different forms depending on the reduced dimension of the carrier gas (cf. Appendix A.2). They are closely related to the functions (1.4), namely the distribution function is

$$f(s) = c\,\mathfrak{F}_\alpha\big(-\frac{s}{\beta}\big), \qquad \alpha = \begin{cases} -1 & \text{if } d = 3, \\ -\frac{1}{2} & \text{if } d = 2, \\ 0 & \text{if } d = 1, \end{cases} \tag{1.12}$$

with positive constants c and β. According to (1.5) the corresponding primitive is

$$F(t) = -\int_t^\infty f(s)ds = -c\beta\,\mathfrak{F}_{\alpha+1}\big(-\frac{t}{\beta}\big). \tag{1.13}$$

More precisely, for an ensemble of electrons in a quantum dot, i.e. $\Omega \subset \mathbb{R}^3$, the distribution function is essentially given by Fermi's function

$$f(s) = 2\,g\,\mathfrak{F}_{-1}\big(-\frac{s}{k_B T}\big) = \frac{2\,g}{1+\exp\big(\frac{s}{k_B T}\big)}, \tag{1.14}$$

k_B being Boltzmann's constant, $T = T_\varsigma$ the temperature of the carrier gas, and $g = g_\varsigma$ a material constant. For the one–dimensional electron gas in a quantum wire, i.e. $\Omega \subset \mathbb{R}^2$, the distribution function is

$$f(s) = 2\,g\sqrt{\frac{m_\perp k_B T}{2\pi\hbar^2}}\,\mathfrak{F}_{-\frac{1}{2}}\big(\frac{-s}{k_B T}\big) = \frac{g}{\pi\hbar}\sqrt{2\,m_\perp k_B T}\int_0^\infty \frac{\xi^{-\frac{1}{2}}}{1+\exp\big(\xi + \frac{s}{k_B T}\big)}\,d\xi, \tag{1.15}$$

and for the two–dimensional electron gas in a quantum well i.e. $\Omega \subset \mathbb{R}^1$ there is

$$(1.16) \qquad f(s) = 2g\frac{m_\perp k_B T}{2\pi\hbar^2}\mathfrak{F}_0\Big(1+\exp\big(\frac{-s}{k_BT}\big)\Big) = g\frac{m_\perp k_B T}{\pi\hbar^2}\ln\Big(1+\exp\big(\frac{-s}{k_BT}\big)\Big),$$

where $m_\perp = m_{\perp\varsigma}$ is the component perpendicular to Ω of the effective–mass tensor of ς–type carriers.

1.1. Remark. The expressions (1.6) and (1.7) 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) and Appendix A.2).

In semiconductor device modeling one has to cope in general with rather complex, mixed boundary conditions [17]. As far as the electrostatic potential φ is concerned, we regard the following ones:

$$(1.17) \qquad 0 = \varphi - \varphi_{\hat\Gamma} \quad \text{on } \hat\Gamma, \quad -\langle \nu, \varepsilon \operatorname{grad} \varphi\rangle = b(\varphi - \varphi_{\hat\Gamma}) \quad \text{on } \partial\hat\Omega \setminus \hat\Gamma,$$

where the function $\varphi_{\hat\Gamma}$, defined on the closure of $\hat\Omega$, represents the boundary values given on $\hat\Gamma$ and the inhomogeneous boundary condition of third kind on $\partial\hat\Omega \setminus \hat\Gamma$. ν denotes the outer unit normal at the boundary $\partial\hat\Omega$ of the device domain $\hat\Omega$ and $\hat\Gamma$ models Ohmic contacts. The part $\partial\hat\Omega \setminus \hat\Gamma$ covers the interface between the semiconductor device and an insulator, where $b \geq 0$ is a capacity, and the rest of $\partial\hat\Omega$, where homogeneous Neumann boundary conditions are prescribed i.e. $b = 0$ (cf. [17]).

How to supplement the Schrödinger operators (1.8) by suitable boundary conditions is a widely discussed question (cf. e.g. [16, 29, 30, 45, 31, 4, 46]). If we assume a device structure which, by confining the charge carrieres, helps to enforce charge neutrality, homogeneous Dirichlet boundary conditions for the eigenfunctions ψ of the Schrödinger operators (1.8) might do the job (cf. [16]). Then the carrier densities vanish on the boundary of Ω and there should be a depletion zone around the device (cf. [29]). Alternatively, one can use homogeneous Neumann boundary conditions. We take into account the following mixed boundary conditions

$$(1.18) \qquad 0 = \psi \quad \text{on } \Gamma, \quad 0 = \langle \nu, m_\varsigma^{-1} \operatorname{grad} \psi\rangle \quad \text{on } \partial\Omega \setminus \Gamma$$

for all ψ in the domain of the Schrödinger operator from (1.8). As T. Kerkhoven pointed out, the envelope–functions defining the carrier densities really shouldn't 'feel' the boundary conditions too much in those parts of the device where one is genuinely interested in the carrier densities.

2. Mathematical formulation of the problem

Mathematically, one has to impose some conditions on the domains $\hat\Omega$ and Ω and on the parts of its boundaries which assure certain regularity properties for the solutions of both, the Poisson and the Schrödinger equation. The problem is here that the mixed boundary conditions together with discontinuous coefficients prevent dom(H) lying in $W^{2,2}$, what is commonly used elsewhere, [36],[26]. Fortunately, it is possible to obtain a reasonable substitute to serve our purpose, at least for the space dimensions up to $d = 3$, which are required for our physical situations. To achieve this, we make the following

2.1. Assumption. $\hat\Omega \subset \mathbb{R}^d$ and $\Omega \subset \hat\Omega$, $1 \leq d \leq 3$, are bounded Lipschitz domains the boundaries $\partial\hat\Omega$ and $\partial\Omega$ of which contain closed Dirichlet parts $\hat\Gamma$ and Γ respectively.

- If the space dimension d is 2, the boundary parts Γ and $\partial\Omega \setminus \Gamma$, satisfy the regularity property of Gröger [22] and the same is true for $\hat{\Gamma}$ and $\partial\hat{\Omega} \setminus \hat{\Gamma}$.
- If $d = 3$ the boundary parts do satisfy the suppositions of Stampaccia [40].

For the convenience of the reader, we quote those results of [22] and [40], which are of interest in the following (for the case $d = 3$, also see [38]). In order to represent the homogeneous Dirichlet boundary conditions we have to introduce adequate subspaces of the spaces $W^{1,p}(\hat{\Omega})$ and $W^{1,p}(\Omega)$:

2.2. Definition. Let $\tilde{\Omega}$ be a Lipschitz domain and $\tilde{\Gamma} \subset \partial\tilde{\Omega}$ be a closed subset of the boundary of $\tilde{\Omega}$ with positive surface measure. Then we denote by $W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega})$ that subspace of the Sobolev space $W^{1,p}(\tilde{\Omega})$ whose elements have a vanishing trace on $\tilde{\Gamma}$ and by $W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega})$ the dual space of $W^{1,p'}_{\tilde{\Gamma}}(\tilde{\Omega})$, $(\frac{1}{p} + \frac{1}{p'} = 1)$. We denote by $\mathcal{J}$ the duality mapping between $W^{1,2}_{\tilde{\Gamma}}(\tilde{\Omega})$ and $W^{-1,2}_{\tilde{\Gamma}}(\tilde{\Omega})$.

2.3. Definition. Let $a : \tilde{\Omega} \longmapsto \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d)$ be a function with positive definite, invertible values, such that $a_u = \|a\|_{L^\infty(\tilde{\Omega},\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}$ and $a_l = \|a^{-1}\|_{L^\infty(\tilde{\Omega},\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}$ are finite. We define the operator $\mathcal{A} : W^{1,2}_{\tilde{\Gamma}}(\tilde{\Omega}) \longmapsto W^{-1,2}_{\tilde{\Gamma}}(\tilde{\Omega})$ by

$$\langle \mathcal{A}v, w\rangle = \int_{\tilde{\Omega}} \langle a(x) \operatorname{grad} v(x), \operatorname{grad} w(x)\rangle + v(x)w(x)\, dx, \quad v, w \in W^{1,2}_{\tilde{\Gamma}}(\tilde{\Omega}).$$

2.4. Theorem. *Let $\tilde{\Omega}$ be a Lipschitz domain and $\tilde{\Gamma} \subset \partial\tilde{\Omega}$ a part, of the boundary such that $\tilde{\Gamma}$ and $\partial\tilde{\Omega} \setminus \tilde{\Gamma}$ satisfy the regularity assumptions of* [22]*. Then*

i) *The function*

$$[2, \infty[\ni p \longmapsto \|\mathcal{J}^{-1}\|_{\mathcal{B}(W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega}))}$$

is monotonously increasing and there is

$$\lim_{p\to 2} \|\mathcal{J}^{-1}\|_{\mathcal{B}(W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega}))} = \|\mathcal{J}^{-1}\|_{\mathcal{B}(W^{-1,2}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,2}_{\tilde{\Gamma}}(\tilde{\Omega}))} = 1.$$

ii) *If $p \geq 2$ and*

$$\frac{a_u - a_l}{a_u + a_l} \|\mathcal{J}^{-1}\|_{\mathcal{B}(W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega}))} < 1 \tag{2.1}$$

then $\mathcal{A}|_{W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega})}$ provides an isomorphism between the spaces $W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega})$ and $W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega})$.

iii) *If one denotes $\mathcal{J}^{-1}|_{W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega})}$ by $\mathcal{J}_p^{-1}$, then one has :*

$$\|\mathcal{A}^{-1}\|_{\mathcal{B}(W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega}))} \leq \frac{a_l}{a_u^2} \frac{\|\mathcal{J}_p^{-1}\|_{\mathcal{B}(W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega}))}}{1 - \frac{a_u - a_l}{a_u + a_l} \|\mathcal{J}_p^{-1}\|_{\mathcal{B}(W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}),W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega}))}}$$

iv) *If for some number $p \geq 2$ (2.1) is satisfied, then for $q = \frac{p}{p-1}$ the mapping $\mathcal{A}^{-1}$ possesses an extension to the space $W^{-1,q}_{\tilde{\Gamma}}(\tilde{\Omega})$, which is isomorphically mapped onto $W^{1,q}_{\tilde{\Gamma}}(\tilde{\Omega})$. Additionally,*

$$\mathcal{A}^{-1} : W^{-1,q}_{\tilde{\Gamma}}(\tilde{\Omega}) \longmapsto W^{1,q}_{\tilde{\Gamma}}(\tilde{\Omega}) \quad \textit{is the adjoint to} \quad \mathcal{A}^{-1} : W^{-1,p}_{\tilde{\Gamma}}(\tilde{\Omega}) \longmapsto W^{1,p}_{\tilde{\Gamma}}(\tilde{\Omega})$$

and, hence, their norms are equal.

2.5. Remark. According to the first assertion of Theorem 2.4 there is always an $\epsilon > 0$, such that (2.1) is satisfied for all $p \in [2, 2 + \epsilon]$.

2.6. Theorem. *Let $\tilde{\Omega}$ again be a Lipschitz domain and $\tilde{\Gamma}$ a part of the boundary $\partial\tilde{\Omega}$ such that $\tilde{\Gamma}$ and $\partial\tilde{\Omega} \setminus \tilde{\Gamma}$ satisfy the suppositions in* [40] *for the mixed boundary value problems. Further, let $\mathcal{A}$ be according to Definition 2.3. Then the mapping $\mathcal{A}^{-1} : W_{\tilde{\Gamma}}^{-1,2}(\tilde{\Omega}) \longmapsto W_{\tilde{\Gamma}}^{1,2}(\tilde{\Omega})$ possesses an extension to the spaces $L^p(\tilde{\Omega}) + \operatorname{div}((L^q(\tilde{\Omega}))^d)$ (where $p > \frac{d}{2}$ and $q > d$) which is mapped thereby continuously into some Hölder space $C^\alpha(\tilde{\Omega})$ with $\alpha > 0$.*

In the following we will frequently use

2.7. Corollary. *Let $\tilde{\Omega}$ be a Lipschitz domain and $\tilde{\Gamma} \subset \partial\tilde{\Omega}$ satisfy the supposition in Theorem 2.4 if $d = 2$ or in Theorem 2.6 if $d = 3$. Then for any $p > \frac{d}{2}$ with $p \geq 1$ the mapping $\mathcal{A}$ of Definition 2.3 has an inverse, which maps $L^p(\tilde{\Omega})$ into a space $C^\alpha(\tilde{\Omega}) \hookrightarrow L^\infty(\tilde{\Omega})$ and which can be extended to a continuous mapping from $L^1(\tilde{\Omega})$ into $L^{p'}(\tilde{\Omega})$, where $\frac{1}{p'} = 1 - \frac{1}{p}$. Further, one has*

$$\|\mathcal{A}^{-1}\|_{\mathcal{B}(L^1(\tilde{\Omega}),L^{p}(\tilde{\Omega}))} = \|\mathcal{A}^{-1}\|_{\mathcal{B}(L^{p'}(\tilde{\Omega}),L^\infty(\tilde{\Omega}))} < \infty.$$

The corollary follows easily Theorem 2.4 or Theorem 2.6, respectively, the selfadjointness of $\mathcal{A}$ on $L^2(\tilde{\Omega})$ and by embedding results.

2.8. Remark. In particular, the Assumption 2.1 on the boundary of Ω assures that the domains (provided with their graph norm) of the Schrödinger operators (cf. Definition 2.12) acting in the Hilbert space $L^2(\Omega)$, continuously embed into a space of Hölder continuous functions. We will make use of this property without further comment in the sequel.

Let us now introduce some further mathematical notions and assumptions, which are necessary for a precise formulation of the Schrödinger–Poisson problem. We will start with the quasi Fermi levels ϕ_ς and the statistical distribution functions $\mathcal{F}_\varsigma$ occuring in (1.2):

2.9. Assumption. The functions ϕ_ς, which represent the quasi Fermi levels, are supposed to be from $W_{\hat{\Gamma}}^{1,2}(\hat{\Omega}) \cap L^\infty(\hat{\Omega})$.

2.10. Assumption. The statistical distribution functions $\mathcal{F}_\varsigma$ are supposed to be monotone and to define locally Lipschitz continuous mappings $F_\varsigma : W_{\hat{\Gamma}}^{1,2}(\hat{\Omega}) \mapsto W_{\hat{\Gamma}}^{-1,2}(\hat{\Omega})$ which are given by

$$\langle F_\varsigma(v), w\rangle = \int_{\hat{\Omega}\setminus\Omega} e_\varsigma \mathcal{F}_\varsigma(e_\varsigma(\phi_\varsigma(x) - v(x)))w(x)\,dx \quad v, w \in W_{\hat{\Gamma}}^{1,2}(\hat{\Omega}). \tag{2.2}$$

2.11. Remark. Sufficient analytic conditions for the functions $\mathcal{F}_\varsigma$ to fulfill Assumption 2.10 are:

- $d = 1$: $\mathcal{F}_\varsigma$ itself is locally Lipschitzian.
- $d = 2$ or $d = 3$: $\mathcal{F}_\varsigma$ is differentiable and the derivative $\mathcal{F}_\varsigma'$ is bounded on $]-\infty, 1]$ and obeys:

  $$|\mathcal{F}_\varsigma'(s)| \leq \delta|s|^p, \quad s \in [1, \infty[,$$

  where p is any finite number if $d = 2$ and a number not greater than 4, if $d = 3$.

Of course, the Fermi Dirac distribution function (1.3), which we have mainly in mind, obeys these conditions.

Next we introduce a precise notion of the Schrödinger operator.

2.12. Definition. For any $\varsigma \in \{1, \dots, \sigma\}$ suppose $m = m_\varsigma \in L^\infty(\Omega, \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d))$ with positive definite, invertible values such that m^{-1} is also from $L^\infty(\Omega, \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d))$. We define the Schrödinger operator with zero potential $H_0 : W_\Gamma^{1,2}(\Omega) \longmapsto W_\Gamma^{-1,2}(\Omega)$ by

$$\langle H_0 v, w\rangle = \frac{\hbar^2}{2} \int_\Omega \left\langle m(x)^{-1} \operatorname{grad} v(x), \operatorname{grad} w(x)\right\rangle dx, \quad v, w \in W_\Gamma^{1,2}(\Omega). \tag{2.3}$$

The restriction of this operator to other range spaces — in particular $L^2(\Omega)$ — we also denote by H_0. However, the notion $\operatorname{dom}(H_0)$ is reserved for the Schrödinger operator in the Hilbert space context of $L^2(\Omega)$. If $p \geq 2$ and $V \in L^p$, then we denote the operator $H_0 + V$ (which is also defined on $\operatorname{dom}(H_0)$, cf. Proposition 3.3) by H_V.

We recall some basic facts on H_0 (cf. e.g. [28] or [39]), which are essential for this paper:

2.13. Theorem. *H_0 is a nonnegative, selfadjoint operator with pure point spectrum. If d is the dimension of the spatial domain, then the resolvents of H_0, are q–summable operators for all $q > \frac{d}{2}$ with $q \geq 1$.*

The proof of the second assertion rests upon the following facts: The eigenvalues of H_0 are lying between the corresponding eigenvalues of the operator $-\frac{\hbar^2}{2} \operatorname{div}(m^{-1} \operatorname{grad})$ once combined with pure (homogeneous) Neumann and on the other hand pure (homogeneous) Dirichlet conditions (cf. Courant/Hilbert [14, ch. VI, $ 2]). The asserted summability property is now an easy consequence of the asymptotics for the eigenvalues of $-\Delta$, both, in case of Dirichlet or Neumann conditions (cf. Courant/Hilbert [14, ch. VI, $ 4]) and the upper and lower bounds for m.

Next we will introduce the class of distribution functions $f = f_\varsigma$, which are admissable in our context. In order to cover all physically relevant cases (cf. §1) and to meet the mathematical requiries for proving our theorems, we make the following assumption:

2.14. Assumption. f is a positive, differentiable, strictly monotonously decreasing function on $\mathbb{R}$. For any $\rho \in \mathbb{R}$ and any

$$k \leq \begin{cases} 3 & \text{if } d = 1, 2, \\ 4 & \text{if } d = 3. \end{cases} \tag{2.4}$$

there is

$$\mathbf{\Lambda}_{k,\rho} = \sup_{s \in [\frac{1}{4}, \infty[} f(s+\rho)s^k < \infty, \qquad \mathbf{\Lambda}'_{k,\rho} = \sup_{s \in [\frac{1}{4}, \infty[} f'(s+\rho)s^{k+1} < \infty. \tag{2.5}$$

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

2.15. Definition. Let f and k be in accordance with Assumption 2.14, and ρ an arbitrary real number We introduce the functions

$$g_{k,\rho} : [0, 4] \longmapsto \mathbb{R}, \qquad g_{k,\rho}(s) = \begin{cases} f\left(s^{-1} + \rho\right) s^{-k} & \text{for } s > 0 \\ 0 & \text{for } s = 0 \end{cases} \tag{2.6}$$

and denote by

$$\boldsymbol{L}_{k,\rho} = \sup_{s \in [0,4]} \left| g'_{k,\rho} \right| \tag{2.7}$$

the corresponding Lipschitz constants which easily can be expressed in terms of the distribution function f.

2.16. Definition. Let f be a distribution function fulfilling Assumption 2.14 and m as in Definition 2.12. Then we define a pseudo carrier density operator corresponding to f and m by

$$\tilde{\mathcal{N}}(V)(x) = \sum_{l=1}^{\infty} f(\mathcal{E}_l(V)) \left|\psi_l(V)(x)\right|^2, \quad V \in L^2(\Omega), \quad x \in \Omega. \tag{2.8}$$

Here the $\mathcal{E}_l(V)$ and $\psi_l(V)$ are the eigenvalues and normalized eigenfunctions, respectively, of the Schrödinger operator $H_V = H_0 + V$. If $\varsigma \in \{1, \dots, \sigma\}$, $f = f_\varsigma$ and $m = m_\varsigma$ then we define the ς–particle density operator $\mathcal{N} = \mathcal{N}_\varsigma$ by

$$\mathcal{N}(V) = \tilde{\mathcal{N}}(V - \mathcal{E}_F(V)) \tag{2.9}$$

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

$$\int_\Omega \mathcal{N}(V)\, dx = \sum_l f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) \; = \; N, \tag{2.10}$$

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

2.17. Remark. We have introduced the notion of the pseudo carrier density operator, (at first excluding the Fermi level), because it serves well our functional analytic purpose. In particular, the reader should note that it is a mapping from suitable function spaces over the domain Ω into spaces of functions, which are again defined over Ω. Later, when we are again regarding the system as a whole, the values of the corresponding carrier densitiy operators will also be regarded as functions over the greater domain $\hat{\Omega}$, embedding them by an operator Z into $L^2(\hat{\Omega})$.

2.18. Remark. A priori it is evident only for potentials $V \in L^\infty(\Omega)$, 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 (2.8) (there V substituted by $V - \mathcal{E}_F(V)$), which defines the particle density operator $\mathcal{N}_\varsigma$, is absolutely converging in $L^1(\Omega)$. Later it will become apparant (cf. Proposition 5.8) that the particle density operators $\mathcal{N}$ are well defined as operators from $L^2(\Omega)$ into spaces of much more regular functions.

2.19. 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 $\left(L^1(\Omega)\right)^\sigma$ into $L^2(\Omega)$ for any $\varsigma \in \{1, \dots, \sigma\}$.

2.20. Remark. In the two– and three–dimensional case the generic exchange–correlation potentials (1.10) belong to that class. This is not true for the one–dimensional case. However, there is still a lot of uncertainty about correct expressions for the exchange–correlation potentials, especially for electron gases with reduced dimension.

2.21. Assumption. The function $\varphi_{\hat{\Gamma}}$, which represents the boundary values given on $\hat{\Gamma}$ and the inhomogeneous boundary condition of third kind on $\partial\hat{\Omega} \setminus \hat{\Gamma}$, is from the space $W^{1,2}(\hat{\Omega})$. Let $\tilde{\varphi}_{\hat{\Gamma}}$ denote the linear form on $W^{1,2}_{\hat{\Gamma}}$, which is given by

$$h \longmapsto \int_{\hat{\Omega}} \langle \varepsilon(x) \operatorname{grad} \varphi_{\hat{\Gamma}}(x), \operatorname{grad} h(x) \rangle \, dx, \quad h \in W^{1,2}_{\hat{\Gamma}}. \tag{2.11}$$

2.22. Definition. Suppose $\varepsilon \in L^\infty(\hat{\Omega}, \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d))$ with positive definite values such that the essential infimum of the lowest eigenvalues is strictly positive. Further, let $0 \le b$ be from $L^\infty(\partial\hat{\Omega} \setminus \hat{\Gamma})$ (with respect to the surface measure), and let either the surface measure of $\hat{\Gamma}$ be not zero or b be strictly positive on a subset of $\partial\hat{\Omega} \setminus \hat{\Gamma}$ with positive surface measure. Then we define the operator $A : W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}) \longmapsto W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})$ by

$$\langle Av, w\rangle = \int_{\hat{\Omega}} \langle \varepsilon(x) \operatorname{grad} v(x), \operatorname{grad} w(x)\rangle \, dx + \int_{\partial\hat{\Omega}\setminus\hat{\Gamma}} b(\tau)v(\tau)w(\tau) \, d\tau, \quad v, w \in W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}).$$

The definition is correct, because $W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})$ embeds continuously into $L^2(\partial\hat{\Omega} \setminus \hat{\Gamma})$.

We denote by c_b a constant such that

$$(2.12) \qquad \|u\|^2_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})} \le c_b\big(\|\operatorname{grad} u\|^2_{L^2(\hat{\Omega},R^d)} + \|bu^2\|_{L^1(\partial\hat{\Omega}\setminus\hat{\Gamma})}\big) \qquad \text{for all} \quad u \in W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}).$$

The constant c_b depends on $\hat{\Omega}$, $\hat{\Gamma}$ and b. Indeed, it is finite as the surface measure of $\hat{\Gamma}$ is nonzero or b does not vanish almost everywhere on $\partial\hat{\Omega} \setminus \hat{\Gamma}$ [19, ch. II, §1, Lemma 1.36].

2.23. Definition. Suppose

$$(2.13) \qquad N_A - N_D \in L^2(\hat{\Omega}), \qquad \Delta E_\varsigma \in L^2(\Omega), \quad \varsigma \in \{1, \dots, \sigma\}$$

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

$$(2.14) \qquad Z_\varsigma : L^2(\hat{\Omega}) \longmapsto L^2(\Omega), \quad \varsigma \in \{1, \dots, \sigma\}.$$

to be given. Further, let $\varepsilon, m_1, \dots, m_\sigma$, f and $\varphi_{\hat{\Gamma}}$ be given and the preceeding assumptions satisfied. We define the external potentials V_ς and the effective doping D by

$$(2.15) \qquad V_\varsigma = Z^*_\varsigma \varphi_{\hat{\Gamma}} - e_\varsigma \Delta E_\varsigma, \quad \varsigma \in \{1, \dots, \sigma\},$$

$$(2.16) \qquad D = q(N_A - N_D) - \tilde{\varphi}_{\hat{\Gamma}}.$$

Then we say that $(V, u_1, ..., u_\sigma) \in W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}) \times L^2(\Omega, \mathbb{R}^\sigma)$ is a solution of the Kohn–Sham system (Schrödinger–Poisson system with exchange–correlation potential) if

$$(2.17) \qquad AV = D + \sum_{\varsigma\in\{1,\dots,\sigma\}} Z^*_\varsigma u_\varsigma + F_\varsigma(V)$$

$$(2.18) \qquad u_\varsigma = \mathcal{N}_\varsigma\left(V_\varsigma + V_{xc,\varsigma}(\mathbf{u}) + Z_\varsigma V\right), \quad \varsigma \in \{1, \dots, \sigma\}.$$

2.24. Remark. With respect to the formulation of the problem in §1, the mapping Z_ς is simply the operator, which restricts functions over $\hat{\Omega}$ to Ω, multiplied by $e_\varsigma q$:

$$(2.19) \qquad (Z_\varsigma v)(x) = e_\varsigma q v(x), \quad x \in \Omega, \qquad \left(Z^*_\varsigma w\right)(x) = \begin{cases} e_\varsigma q w(x), & x \in \Omega, \\ 0 \quad , & x \in \hat{\Omega} \setminus \Omega. \end{cases}$$

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 6.5, the class of admissable operators may be widened by small perturbations.

2.25. Remark. The natural space for the quantum mechanical particle densities u_ς, (2.9), to ly in is $L^1(\Omega)$, because the charge conservation laws (2.10) accord to this space. But the functional anlytic context, in which we will regard the system, is mainly determined by the monotonicity properties of the nonlinear Poisson operator, acting between $W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})$ and $W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})$. Thus, we have decided to associate with the notion of a solution that the particle densities are also from $L^2(\Omega)$. In fact, it turns out later (see Remark 6.15) that the structure of the system itself assures that the particle densities are much more regular over Ω, even when at first only $u_\varsigma \in L^1(\Omega)$ is supposed. It should be noted, however, that on the boundary of Ω discontinuities of the carrier densities may appear. This depends on the fact that in the present concept the densities u_ς within the quantum mechanically described region Ω and in the macroscopically described one are related only via the nonlinear Poisson equation, i.e. the electrostatic potential φ. A completely selfconsistent approach would have to include equations for the — macroscopic and microscopic — Fermi level, a program which we will carry out in later papers [24, 25].

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

2.26. Theorem. *(cf.* [19, ch. III, §3.2]*.) Let* A *be a strongly monotone and boundedly Lipschitz continuous operator between the Hilbert space* H *and its dual* H^**. Then the equation*

$$\mathrm{A}(\mathrm{u}) = \mathrm{f} \tag{2.20}$$

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

$$\|\mathrm{u}\|_H \le \frac{1}{m_{\mathrm{A}}} \|\,\mathrm{A}(0) - \mathrm{f}\|_{H^*}, \tag{2.21}$$

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

$$\frac{2}{m_{\mathrm{A}}} \|\,\mathrm{A}(0) - \mathrm{f}\|_{H^*}. \tag{2.22}$$

Then the operator

$$\mathrm{u} \to \mathrm{u} - \frac{m_{\mathrm{A}}}{M_{\mathrm{A}}^2} J^{-1}\big(\mathrm{A}(\mathrm{u}) - \mathrm{f}\big) \tag{2.23}$$

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

$$\sqrt{1 - \frac{m_{\mathrm{A}}^2}{M_{\mathrm{A}}^2}}. \tag{2.24}$$

The fixed point of (2.23) *is identical with the solution of* (2.20)*.*

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

2.27. Theorem. *Let* $S = [0, a]$ *be any finite interval and* g *any 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*

$$\|g(\mathrm{B})\|_q \le \mathbf{Lip}_S(g)\,\|\,\mathrm{B}\,\|_q, \tag{2.25}$$

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

$$\|\mathrm{B}^\alpha\|_{\frac{q}{\alpha}} = \|\mathrm{B}\|_q^\alpha, \quad 1 \le q < \infty, \quad 0 < \alpha \le q. \tag{2.26}$$

2.28. Theorem. *(Birman and Solomjak* [7, 8]*.) Let* A *and* B *be two selfadjoint operators, whose difference is Hilbert–Schmidt and whose spectral measures are concentrated on a finite interval* $S \subset \mathbb{R}$*. Further, assume that* $g : S \longmapsto \mathbb{R}$ *is Lipschitz continuous on* S *with the Lipschitz constant* $\mathbf{Lip}_S(g)$*. Then one has*

$$\|g(\mathrm{A}) - g(\mathrm{B})\|_2 \;\le\; \mathbf{Lip}_S(g)\,\|\,\mathrm{A} - \mathrm{B}\,\|_2. \tag{2.27}$$

Finally we cite two deep complex interpolation results, which we use to get fine tuned estimates later on.

2.29. Theorem. *(cf.* [42, Section 1.15.3]*.) If* B *is a strictly positive, selfadjoint operator, then*

$$[\mathrm{dom}(\mathrm{B}^{\delta}), \mathrm{dom}(\mathrm{B}^{\beta})]_{\Theta} = \mathrm{dom}(\mathrm{B}^{\delta(1-\Theta)+\beta\Theta}), \quad 0 < \Theta < 1, \quad 0 \le \Re\delta < \Re\beta < \infty. \tag{2.28}$$

2.30. Theorem. *(cf.* [42, Section 4.3.1]*.) If $\tilde{\Omega}$ is a domain satisfying a cone condition, then*

$$\left[W^{1,p}(\tilde{\Omega}), W^{1,q}(\tilde{\Omega})\right]_{\Theta} = W^{1,r}(\tilde{\Omega}), \qquad \textit{(including the equivalence of norms)} \tag{2.29}$$

$$0 < \Theta < 1, \quad 1 < p, q < \infty, \quad \frac{1}{r} = \frac{1-\Theta}{p} + \frac{\Theta}{q}.$$

3. The Schrödinger operator with mixed boundary conditions

In this section we present properties of the Schrödinger operator which are afterwards an essential instrument for verifying the existence and uniqueness statements for the Schrödinger–Poisson system. For the sake of technical simplicity, during this and the next chapter we will often omit the symbol Ω in the notation of function spaces, because all of them are belonging to Ω. — m has to be regarded as any of the effective masses m_ς, $\varsigma \in \{1, \dots, \sigma\}$. In the following propositions, certain Gagliardo–Nirenberg constants and the L^∞–bound of m play an essential role.

3.1. Definition. If the dimension of the spatial domain equals d we define γ_p as the Gagliardo–Nirenberg constant (cf. e.g. [34, 1.4.8/1])

$$\gamma_p = \sup_{0 \ne \psi \in W_\Gamma^{1,2}} \frac{\|\psi\|_{L^{\frac{2p}{p-1}}}}{\|\psi\|_{W_\Gamma^{1,2}}^{\frac{d}{2p}} \cdot \|\psi\|_{L^2}^{1-\frac{d}{2p}}}, \qquad p \ge 1, \quad p > \frac{d}{2}. \tag{3.1}$$

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

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

3.2. Remark. $\overline{m}$ has been defined such that $\frac{1}{\overline{m}}$ is the monotonicity constant of the operator $(H_0 + 1) : W_\Gamma^{1,2} \to W_\Gamma^{-1,2}$, (cf. Definition 2.12), hence, $\overline{m}$ is the norm of the inverse operator:

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

Now we regard the Schrödinger operator

$$H = H_V = H_0 + V \tag{3.4}$$

from Definition 2.12 in the Hilbert space $L^2(\Omega)$.

3.3. Proposition. *Let V be from $L^p(\Omega)$, $p \ge 2$. One has:*

i) *V, as a multiplication operator acting on the Hilbert space $L^2(\Omega)$, is infinitesimally small and relatively compact with respect to $H_0 + 1$. Hence, if V is real–valued, then $H_V = H_0 + V$ is again selfadjoint and has, as well as H_0, a pure point spectrum. The eigenfunctions ψ_l of H_V form an orthonormal basis in $L^2(\Omega)$ and all eigenvalues are real.*

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

$$(3.5)\quad 1-\frac{d}{2p}+\rho_V \le (1-\frac{d}{2p})(H_0+1)+\rho_V \le\ H_0+V\ \le (1+\frac{d}{2p})(H_0+1)-\rho_V-2,$$

where

$$(3.6)\qquad \rho_V=-\big(1-\frac{d}{2p}\big)\|V\|_{L^p}^{\frac{2p}{2p-d}}\,\gamma_p^{\frac{4p}{2p-d}}\,\overline{m}^{\frac{d}{2p-d}}-1.$$

iii) *If $\rho \le \rho_V$, then the spectrum of $(H_V-\rho)^{-1}$ is contained in $[0,4]$ and*

$$(3.7)\qquad \|(H_V-\rho)^{-\frac12}(H_0+1)^{\frac12}\|=\|(H_0+1)^{\frac12}(H_V-\rho)^{-\frac12}\|\le(1-\frac{d}{2p})^{-\frac12}.$$

iv) *For any $V\in L^2(\Omega)$ and any q with $q\ge 1$ and $q>\frac{d}{2}$ the resolvent of H_V is a q–summable operator and one has*

$$(3.8)\qquad \|(H_V-\rho)^{-1}\|_q\le(1-\frac{d}{2p})^{-1}\|(H_0+1)^{-1}\|_q<\infty,\quad \rho\le\rho_V.$$

3.4. Remark. The lower form bound of H_0+V in (3.5) 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 (3.5).

Proof of i). Because $L^p \hookrightarrow L^2$ if $p>2$ we may focus our attention to the case $V\in L^2(\Omega)$. First we prove that V has then zero bound with respect to H_0+1. Because the embedding $C^\alpha(\Omega)\hookrightarrow L^\infty(\Omega)$ is compact and the embedding $L^\infty(\Omega)\hookrightarrow L^2(\Omega)$ is injective, one may apply Ehrling's lemma (cf. e.g. Wloka [47]). That means, for any ϵ there is a $\delta(\epsilon)$ such that for any $\psi\in\mathrm{dom}(H_0)$ there is

$$\|V\psi\|_{L^2}\le\|V\|_{L^2}\,\|\psi\|_{L^\infty}\le\|V\|_{L^2}(\epsilon\,\|\psi\|_{C^\alpha}+\delta(\epsilon)\|\psi\|_{L^2})$$

Then the term $\|\psi\|_{C^\alpha}$ may be estimated by $\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,C^\alpha)}\,\|(H_0+1)\psi\|_{L^2}$ (cf. Remark 2.8) what proves the first assertion. The relative compactness results from the continuity of the embedding $\mathrm{dom}(H_0)\hookrightarrow C^\alpha$ and the compactness of the embedding $C^\alpha\hookrightarrow L^\infty$. — The discreteness of the spectrum of H_V follows from the compactness of the resolvent of H_0 and the invariance of the essential spectrum under relative compact perturbations (cf. Kato [28]). The last assertion is a wellknown fact on selfadjoint operators with pure point spectrum [28]. □

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

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

We estimate the form

$$W_\Gamma^{1,2}\ni\psi\longmapsto\langle|V|\psi,\psi\rangle$$

beginning with an application of Hölder's inequality:

$$\langle|V|\psi,\psi\rangle\le\|V\|_{L^p}\|\psi\|^2_{L^{\frac{2p}{p-1}}}$$

then the Gagliardo–Nirenberg inequality

$$\le\|V\|_{L^p}\,\gamma_p^2\,\Big(\|\psi\|^2_{W_\Gamma^{1,2}}\Big)^{\frac{d}{2p}}\,\|\psi\|_{L^2}^{2-\frac{d}{p}}$$

(3.3)

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

and finally Young's inequality

$$\leq \frac{d}{2p}\langle (H_0+1)\psi,\psi\rangle + (1-\frac{d}{2p})\|V\|_{L^p}^{\frac{2p}{2p-d}}\,\gamma_p^{\frac{4p}{2p-d}}\,m^{\frac{d}{2p-d}}\,\|\psi\|_{L^2}^2$$
$$= \left\langle \left(\frac{d}{2p}(H_0+1) +\ (1-\frac{d}{2p})\ \|V\|_{L^p}^{\frac{2p}{2p-d}}\,\gamma_p^{\frac{4p}{2p-d}}\,m^{\frac{d}{2p-d}}\right)\psi,\psi\right\rangle.$$

□

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

$$\|(H_V-\rho_V)^{\frac12}(H_V-\rho)^{-\frac12}\|\leq 1$$

(cf. [28, ch. VI, §2]). From (3.5) and the definition of ρ_V follows that

$$\frac{1}{4}(H_0+1)\leq(1-\frac{d}{2p})(H_0+1)\leq H_V-\rho_V \tag{3.9}$$

is true in the sense of forms. Consequently, the spectrum of $H_V-\rho_V$ has to ly above $\frac14$, and — by the spectral mapping theorem — the spectrum of $(H_V-\rho_V)^{-1}$ is localized in the interval $[0,4]$. — For $\rho=\rho_V$ (3.7) follows from (3.9), [28, ch. VI, §2], and the fact that the operators $(H_V-\rho)^{-\frac12}(H_0+1)^{\frac12}$ and $(H_0+1)^{\frac12}(H_V-\rho)^{-\frac12}$ are adjoint to each other. □

Proof of iv). (3.8) is trivially implied by (3.7) and Theorem 2.13. □

3.5. Remark. N.B. the conditions $p>\frac{d}{2}$ and $p\geq 1$ restrict the following considerations to the space dimensions $d=1,2,3$, because the adequate sets of potentials are bounded in $L^2(\Omega)$ only (see also Remark 6.16).

3.6. Corollary. *From* (3.5) *and the minimax principle (cf. e.g. Reed, Simon* [39]*) one gets the following estimate for the eigenvalues $\mathcal{E}_l(V)$ of the operator $H_V=H_0+V$:*

$$(1-\frac{d}{2p})(\lambda_l+1)+\rho_V\leq\ \mathcal{E}_l(V)\ \leq(1+\frac{d}{2p})(\lambda_l+1)-\rho_V-2,\quad l=1,2,\dots \tag{3.10}$$

where the λ_l are the eigenvalues of the operator H_0, and ρ_V is according to (3.6).

3.7. Proposition. *Suppose $V\in L^2(\Omega)$ and real–valued. Then the graph norms of H_0 and H_V on $L^2(\Omega)$ are equivalent. If ρ is a lower bound of $H_V-(1-\frac{d}{4})$, then one has in the case $d=1$*

$$\begin{aligned}\|(H_0+1)(H_V-\rho)^{-1}\|\leq 1&+(\|V\|_{L^2}+|\rho+1|\,|\Omega|^{\frac12})\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)}\\&+\frac43(\|V\|_{L^2}+|\rho+1|\,|\Omega|^{\frac12})^2\|(H_0+1)^{-1}\|^2_{\mathcal{B}(L^1,L^\infty)}<\infty,\end{aligned} \tag{3.11}$$

in the case $d=2$

$$\begin{aligned}\|(H_0+1)(H_V-\rho)^{-1}\|\leq&\left[1+(\|V\|_{L^2}+|\rho+1|\,|\Omega|^{1/2})\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)}\right]^2\\&+2(\|V\|_{L^2}+|\rho+1|\,|\Omega|^{\frac12})^3\,\|(H_0+1)^{-1}\|^2_{\mathcal{B}(L^{\frac43},L^\infty)}<\infty,\end{aligned} \tag{3.12}$$

and in the case $d=3$

$$\begin{aligned}\|(H_0+1)(H_V-\rho)^{-1}\|\leq&\left[1+(\|V\|_{L^2}+|\rho+1|\,|\Omega|^{1/2})\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)}\right]^4\\&+4(\|V\|_{L^2}+|\rho+1|\,|\Omega|^{\frac12})^5\,\|(H_0+1)^{-1}\|^4_{\mathcal{B}(L^{\frac85},L^\infty)}<\infty.\end{aligned} \tag{3.13}$$

Proof. The first statement follows from the identity of $dom(H)$ and $dom(H_V)$, the (obvious) continuity of the embedding $dom(H_0) \hookrightarrow dom(H_V)$ and the open mapping theorem; it may also be deduced from the next assertions. For the proof of (3.11), (3.12) and (3.13) we use the formula

$$(3.14) \qquad (H_0+1)(H_V-\rho)^{-1} = \sum_{k=0}^{r} \left[\tilde{V}(H_0+1)^{-1}\right]^k + \left[\tilde{V}(H_0+1)^{-1}\right]^r \tilde{V}(H_V-\rho)^{-1},$$

where

$$(3.15) \qquad \tilde{V} = (H_0+1)-(H_V-\rho) = 1-V+\rho, \quad \|\tilde{V}\|_{L^2} \le \|V\|_{L^2} + |\rho+1|\,|\Omega|^{\frac{1}{2}}.$$

Because ρ has a distance of at least $1-\frac{d}{4}$ to the spectrum of H_V, there is

$$(3.16) \qquad \|(H_V-\rho)^{-1}\| \le (1-\frac{d}{4})^{-1}.$$

For the case $d=1$ we use (3.14) with $r=1$ and estimate thereby using (3.16)

$$(3.17) \quad \|(H_0+1)(H_V-\rho)^{-1}\| \le 1 + \|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)} + \frac{4}{3}\|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^1,L^\infty)}\|\tilde{V}\|_{L^2}.$$

It is easy to see from the continuity of the embeddings $W^{1,2}_\Gamma \hookrightarrow L^\infty$ and $L^1 \hookrightarrow W^{-1,2}_\Gamma$ that $\|(H_0+1)^{-1}\|_{\mathcal{B}(L^1,L^\infty)}$ is finite in the one–dimensional case. Finally, taking into account (3.15), one obtains (3.11).

In the case $d=2$ we use (3.14) with $r=2$ and estimate again using (3.16)

$$(3.18) \quad \|(H_0+1)(H_V-\rho)^{-1}\| \le 1 + \|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)} + \|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)}\|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^2,L^\infty)} + 2\|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^{\frac{4}{3}},L^\infty)}\|\tilde{V}\|_{L^2}\|(H_0+1)^{-1}\|_{\mathcal{B}(L^1,L^4)}\|\tilde{V}\|_{L^2}.$$

By Theorem 2.4 and Sobolev's embedding theorem, $\|(H_0+1)^{-1}\|_{\mathcal{B}(L^1,L^4)}$ is finite, and from the selfadjointness of H_0 on $L^2(\Omega)$ and a simple duality argument

$$\|(H_0+1)^{-1}\|_{\mathcal{B}(L^1,L^4)} = \|(H_0+1)^{-1}\|_{\mathcal{B}(L^{\frac{4}{3}},L^\infty)}$$

follows. Taking into account (3.15), this proves (3.12).

In the case $d=3$ we use (3.14) with $r=4$. Observing (3.15), (3.16), and abbreviating $H_1 = H_0+1$ we estimate the items of the sum in (3.14) by means of

$$\left\|\tilde{V}H_1^{-1}\right\| \le \left(\|V\|_{L^2} + |\rho+1|\,|\Omega|^{\frac{1}{2}}\right)\,\|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)}$$

and

$$\left\|\left[\tilde{V}(H_0+1)^{-1}\right]^4\tilde{V}(H_V-\rho)^{-1}\right\| \le 4\left\|\left[\tilde{V}H_1^{-1}\right]^4\tilde{V}\right\| \le$$

$$4\|\tilde{V}\|_{L^2}\|H_1^{-1}\|_{\mathcal{B}(L^{\frac{8}{5}},L^\infty)}\|\tilde{V}\|_{L^2}\|H_1^{-1}\|_{\mathcal{B}(L^{\frac{4}{3}},L^8)}\|\tilde{V}\|_{L^2}\|H_1^{-1}\|_{\mathcal{B}(L^{\frac{8}{7}},L^4)}\|\tilde{V}\|_{L^2}\|H_1^{-1}\|_{\mathcal{B}(L^1,L^{\frac{8}{3}})}\|\tilde{V}\|_{L^2}$$

To finish the proof of (3.13), one has to give bounds of the factors $\|H_1^{-1}\|_{\mathcal{B}(L^s,L^t)}$. At first one observes that

$$(3.19) \qquad H_1^{-1} : L^{\frac{8}{5}}(\Omega) \longmapsto L^\infty(\Omega)$$

is the adjoint to

$$(3.20) \qquad H_1^{-1} : L^1(\Omega) \longmapsto L^{\frac{8}{3}}(\Omega)$$

and, hence, their norms are equal and finite, cf. Corollary 2.7. Both,

$$H_1^{-1} : L^{\frac{4}{3}}(\Omega) \longmapsto L^8(\Omega) \qquad \text{and} \qquad H_1^{-1} : L^{\frac{8}{7}}(\Omega) \longmapsto L^4(\Omega)$$

are interpolating operators of (3.19) and (3.20), thus their norms are not greater than

$$\|H_1^{-1}\|_{\mathcal{B}(L^{\frac{8}{5}},L^\infty)} = \|H_1^{-1}\|_{\mathcal{B}(L^1,L^{\frac{8}{3}})}$$

by the Riesz–Thorin interpolation theorem. □

3.8. Remark. Because $(H_V-\rho)^{-1}(H_0+1)$ is the adjoint operator to $(H_0+1)(H_V-\rho)^{-1}$, they are equal in norm. We will make use of this frequently in the sequel without further comment.

3.9. Remark. If ρ is a strict lower bound of the operator H_V, one also obtains an estimate for the operator norm of $(H_0+1)(H_V-\rho)^{-1}$, namely

$$\begin{aligned} (3.21)\quad & \|(H_V-\rho)^{-1}(H_0+1)\| \\ & \leq \|(H_V-\rho)^{-1}(H_V-(\rho-1))\| \, \|(H_V-(\rho-1))^{-1}(H_0+1)\| \\ & \leq \left(1+\mathrm{dist}(\rho, \mathrm{spec}[H_V])^{-1}\right) \left\|(H_V-(\rho-1))^{-1}(H_0+1)\right\| \end{aligned}$$

Hence, if a $L^2(\Omega)$–bounded set of Schrödinger potentials is given, and ρ is a uniform strict lower bound for all the corresponding operators H_V, then the norms of the operators $(H_0+1)(H_V-\rho)^{-1}$ and $(H_V-\rho)^{-1}(H_0+1)$ are uniformely bounded with respect to this set. Often this insight completely suffices. We give explicit bounds here, because later on we aim at a–priori bounds in terms of the data for the solutions of the Schrödinger–Poisson system.

We conclude this section with some further properties of the Schrödinger operators (3.4) with potentials V ranging in a $L^2(\Omega)$–bounded set $\mathcal{M}$.

3.10. Lemma. *Assume $\mathcal{M} \subset L^2(\Omega)$ to be bounded and*

$$(3.22)\qquad \rho \leq \rho_{\mathcal{M}} = \sup_{V\in\mathcal{M}} \rho_V\big|_{p=2} = -\big(1-\frac{d}{4}\big)\gamma_2^{\frac{8}{4-d}}\overline{m}^{\frac{d}{4-d}} \sup_{V\in\mathcal{M}} \|V\|_{L^2}^{\frac{4}{4-d}} - 1$$

to be given, where $\rho_V\big|_{p=2}$ is (3.6) with $p=2$, and γ_2, $\overline{m}$ according to Definition 3.1.

i) *If $\{V_n\}_n$ is a sequence from $\mathcal{M}$, $L^2(\Omega)$–weakly converging to V, then the resolvents of H_{V_n} at the point ρ are converging to the resolvent of H_V at ρ in the Hilbert—Schmidt topology, and, hence, in the usual uniform operator topology.*
Consequently, the operators H_{V_n} are converging to H_V in the generalized sense and any finite system of eigenvalues of H_{V_n} is converging to the corresponding finite system of H_V.

ii) *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*

$$(3.23)\qquad (1-\frac{d}{4})^{-2}\|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma,L^4)}\,\overline{m}\,\|(H_0+1)^{-1}\|_2.$$

Proof of i). We prove the first part of the assertion, the second one follows suit by well known theorems (cf. Kato [28, ch. IV $2 and $3]). The Hilbert—Schmidt property of the resolvents follows from Theorem 2.13 and item *iv)* of Proposition 3.3. Because of

$\|V\|_{L^2(\Omega)} \le \sup_n \|V_n\|_{L^2(\Omega)}$, ρ is a lower bound of $H_V - \left(1-\frac{d}{4}\right)$, hence, ρ is in the resolvent set of H_V There is (abbreviating $H_1 = H_0 + 1$)

$$\begin{aligned}\|(H_V-\rho)^{-1}-(H_{V_n}-\rho)^{-1}\|_2 &= \|(H_V-\rho)^{-1}(V_n-V)(H_{V_n}-\rho)^{-1}\|_2\\ &\le \|(H_V-\rho)^{-1}H_1\|\,\|H_1^{-1}(V_n-V)H_1^{-1}\|_2 \sup_n \|H_1(H_{V_n}-\rho)^{-1}\|\\ &\le \|(H_V-\rho)^{-1}H_1\|\,\|H_1^{-4/5}\|_2\,\|H_1^{-1/5}(V_n-V)H_1^{-1}\| \sup_n \|H_1(H_{V_n}-\rho)^{-1}\|\end{aligned}$$

According to Proposition 3.7 the terms $\|(H_V-\rho)^{-1}H_1\|$ and $\sup_n \|H_1(H_{V_n}-\rho)^{-1}\|$ are finite, and so is $\|H_1^{-4/5}\|_2$ by Proposition 3.3 and (2.26). Now it is sufficient to show that

$$\|(H_0+1)^{-1/5}(V_n-V)(H_0+1)^{-1}\| \to 0, \quad \text{as } n\to\infty.$$

Assuming that this is not the case, there is a $\delta > 0$, a subsequence $\{V_k\}_k$ and a sequence $\{\psi_k\}_k$ of normalized elements from $L^2(\Omega)$, such that

$$(3.24) \qquad \|(H_0+1)^{-1/5}(V_k-V)(H_0+1)^{-1}\psi_k\|_{L^2} \ge \delta \qquad \text{for all } k.$$

Because $\operatorname{dom}(H_0)$ (in the graph norm) is compactly embedded into $L^\infty(\Omega)$ (cf. Remark 2.8), the sequence $\{(H_0+1)^{-1}\psi_k\}_k$ contains a subsequence $\{(H_0+1)^{-1}\psi_r\}_r$, which is strongly converging in $L^\infty(\Omega)$. Using this, it is not difficult to see that the sequence $\{(V_r-V)(H_0+1)^{-1}\psi_r\}_r$ is weakly converging in $L^2(\Omega)$ to zero. But $(H_0+1)^{-1/5}$ maps $L^2(\Omega)$ compactly into itself, hence

$$\left\{(H_0+1)^{-1/5}(V_r-V)(H_0+1)^{-1}\psi_r\right\}_r$$

contains a subsequence which converges strongly to zero in $L^2(\Omega)$, and this contradicts (3.24). □

Proof of ii). We start with the following inequality (abbreviating again $H_1 = H_0+1$):

$$(3.25) \quad \begin{aligned}\|(H_V-\rho)^{-1}-(H_U-\rho)^{-1}\|_2 &= \|(H_V-\rho)^{-1}(U-V)(H_U-\rho)^{-1}\|_2\\ &\le \|H_1^{-\frac12}\|_4\|H_1^{\frac12}(H_V-\rho)^{-\frac12}\|\,\|(H_V-\rho)^{-\frac12}H_1^{\frac12}\|\,\|H_1^{-\frac12}(U-V)H_1^{-\frac12}\|\\ &\quad\cdot\|H_1^{\frac12}(H_U-\rho)^{-\frac12}\|\,\|(H_U-\rho)^{-\frac12}H_1^{\frac12}\|\,\|H_1^{-\frac12}\|_4.\end{aligned}$$

Now applying (3.7) and observing (2.26) one gets

$$(3.26) \quad \begin{aligned}&\|(H_U-\rho)^{-1}-(H_V-\rho)^{-1}\|_2\\ &\le (1-\frac{d}{4})^{-2}\|H_1^{-1}\|_2\|H_1^{-\frac12}(U-V)H_1^{-\frac12}\|\\ &\le (1-\frac{d}{4})^{-2}\|H_1^{-1}\|_2\|H_1^{-\frac12}\|_{\mathcal{B}(L^{\frac43},L^2)}\|(U-V)\|_{L^2}\|H_1^{-\frac12}\|_{\mathcal{B}(L^2,L^4)}\\ &= (1-\frac{d}{4})^{-2}\|H_1^{-1}\|_2\|(U-V)\|_{L^2}\|H_1^{-\frac12}\|^2_{\mathcal{B}(L^2,L^4)}.\end{aligned}$$

$\|H_1^{-\frac12}\|_{\mathcal{B}(L^2,L^4)}$ is not greater than the product of $\|H_1^{-\frac12}\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)}$ and the embedding constant $\|\mathbb{1}\|_{\mathcal{B}\left(W^{1,2}_\Gamma\hookrightarrow L^4\right)}$ of $W^{1,2}_\Gamma$ into L^4, which is finite for the space dimensions we consider. Finally, it is not difficult to see (cf. Remark 3.2), that

$$(3.27) \qquad \|H_1^{-\frac12}\|_{\mathcal{B}(W^{-1,2}_\Gamma,L^2)} = \|H_1^{-\frac12}\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)} = \|H_1^{-1}\|^{\frac12}_{\mathcal{B}(W^{-1,2}_\Gamma,W^{1,2}_\Gamma)} \le \overline{m}^{\frac12}.$$

□

In the next propositions we develope some tools which we need for the existence proof later on. 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 [26] and use the embedding of the eigenvalues of $H_0 + V$, given by Corollary 3.6, instead. Moreover, these proofs provide a priori bounds for the solution in terms of the data of the problem.

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

4.1. Lemma. *Let $\mathcal{M} \subset L^2(\Omega)$ be bounded. For any two elements U, V of $\mathcal{M}$, and any $\varsigma \in \{1, \dots, \sigma\}$ a distribution function f from Assumption 2.14 of the Schrödinger operator from Definition 2.12 complies*

(4.1)

$$\left\|f(H_U) - f(H_V)\right\|_1 \leq 2\left(1 - \frac{d}{4}\right)^{-3} \boldsymbol{L}_{1,\rho_{\mathcal{M}}} \, \|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_\Gamma, L^4)} \, \overline{m} \, \|(H_0 + 1)^{-1}\|_2^2 \|U - V\|_{L^2},$$

where $\boldsymbol{L}_{1,\rho_{\mathcal{M}}}$ is the Lipschitz constant from Definition 2.15, and $\rho_{\mathcal{M}}$ is the number (3.22).

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

$$\begin{aligned} \left\|f(H_U) - f(H_V)\right\|_1 &\leq \left\|f(H_U)(H_U - \rho)\right\|_2 \left\|(H_U - \rho)^{-1} - (H_V - \rho)^{-1}\right\|_2 \\ &\quad + \left\|f(H_U)(H_U - \rho) - f(H_V)(H_V - \rho)\right\|_2 \left\|(H_V - \rho)^{-1}\right\|_2. \end{aligned} \tag{4.2}$$

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 2.27 and the Birman–Solomjak Theorem 2.28 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 (2.6). Indeed, this is justified by Proposition 3.3 item *iii)*, because the spectrum of $(H_W - \rho)^{-1}$ is contained in $[0, 4]$ for all $W \in \mathcal{M}$. Consequently Theorem 2.27 yields

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

Correspondingly we get with Theorem 2.28

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

Hence (4.2) may be majorized by

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

Now one can estimate $\left\|(H_U - \rho)^{-1}\right\|_2$ and $\left\|(H_V - \rho)^{-1}\right\|_2$ by means of (3.8), and the term $\left\|(H_U - \rho)^{-1} - (H_V - \rho)^{-1}\right\|_2$ by means of Lemma 3.10 item *ii* using the Lipschitz constant (3.23). □

4.2. Proposition. *Let $\Omega \subset \mathbb{R}^d$ be according to Assumption 2.1. For any $\varsigma \in \{1, \dots, \sigma\}$ we regard the Schrödinger operators $H_V = H_0 + V$ from Definition 2.12 and the Fermi level $\mathcal{E}_F = \mathcal{E}_{F,\varsigma}$ from Definition 2.16.*

i) *For all $V \in L^2(\Omega)$ and any $U \in L^\infty(\Omega)$ there is*

$$|\mathcal{E}_F(V+U) - \mathcal{E}_F(V)| \leq \|U\|_{L^\infty}. \tag{4.3}$$

ii) *Let $\{\lambda_l\}$ be the sequence of eigenvalues of the free Hamiltonian H_0. We define for any $p > \frac{d}{2}$ the numbers $\underline{\epsilon}_p$ and $\bar{\epsilon}_p$ by*

$$\sum_{l=1}^{\infty} f\Big(\big(1 - \frac{d}{2p}\big)\lambda_l - \underline{\epsilon}_p\Big) \;=\; \sum_{l=1}^{\infty} f\Big(\big(1 + \frac{d}{2p}\big)\lambda_l - \bar{\epsilon}_p\Big) \;=\; N, \tag{4.4}$$

where N is as in (2.10). If $V \in L^p(\Omega)$, $p > \frac{d}{2}$ and $p \geq 1$, then one has the following bounds for the Fermi level $\mathcal{E}_F(V)$:

$$\underline{\epsilon}_p + \rho_V + \big(1 - \frac{d}{2p}\big) \leq \mathcal{E}_F(V) \leq \bar{\epsilon}_p - \rho_V - \big(1 - \frac{d}{2p}\big) \tag{4.5}$$

where ρ_V is (3.6).

iii) *$V \mapsto \mathcal{E}_F(V)$ is a Lipschitz continuous mapping $\mathcal{E}_F : L^2(\Omega) \mapsto \mathbb{R}$ on bounded subsets of $L^2(\Omega)$.*

Proof of i). (4.3) follows from the strict decay of f (cf. Assumption 2.14) and the form inequality

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

which implies a corresponding inequality for the eigenvalues. □

Proof of ii). We prove the left part of (4.5), the other runs along the same lines. Assume the opposite, namely

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

This and (3.5) in Proposition 3.3 would imply

$$\big(1 - \frac{d}{2p}\big) H_0 - \underline{\epsilon}_p < H_0 + V - \mathcal{E}_F(V)$$

in the sense of forms. Then from the minimax principle one could conclude the corresponding inequality for the eigenvalues of the operators $(1-\frac{d}{2p})H_0 - \underline{\epsilon}_p$ and $H_0 + V - \mathcal{E}_F(V)$, which is a contradiction to the definitions (4.4) and (1.11) of $\underline{\epsilon}_p$ and $\mathcal{E}_F(V)$, respectively. □

Proof of iii). Let $\mathcal{M} \subset L^2(\Omega)$ be bounded and

$$\widetilde{\mathcal{M}} = \mathcal{M} + \mathcal{E}_F(\mathcal{M})\chi_\Omega,$$

where χ_Ω is the characteristic function of the domain Ω. $\widetilde{\mathcal{M}}$ is bounded due to (4.5). Choose any two elements U, V of $\mathcal{M}$, then we may estimate:

$$\big|\mathcal{E}_F(U) - \mathcal{E}_F(V)\big| \leq \delta_{\mathcal{M}} \Big| f\big(\mathcal{E}_1(V) - \mathcal{E}_F(V)\big) - f\big(\mathcal{E}_1(V) - \mathcal{E}_F(U)\big)\Big| \tag{4.6}$$

where

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

$\delta_{\mathcal{M}}$ can be estimated using the bounds for $\mathcal{E}_1(V)$ established in Corollary 3.6 and the bounds (4.5) 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 2.14) follows that $\delta_{\mathcal{M}}$ is finite.

We continue (4.6) by further enlarging the right hand side:

$$\begin{aligned}\left|\mathcal{E}_F(U)-\mathcal{E}_F(V)\right| &\le \delta_{\mathcal{M}}\left|f\big(\mathcal{E}_1(V)-\mathcal{E}_F(V)\big)-f\big(\mathcal{E}_1(V)-\mathcal{E}_F(U)\big)\right|\\ &\le \delta_{\mathcal{M}}\left|\operatorname{tr}\Big[f\big(H_V-\mathcal{E}_F(V)\big)-f\big(H_V-\mathcal{E}_F(U)\big)\Big]\right|\end{aligned}$$

N.B. $N=\operatorname{tr}\big[f(H_V-\mathcal{E}_F(V))\big]=\operatorname{tr}\big[f(H_U-\mathcal{E}_F(U))\big]$ according to (2.10)

$$\begin{aligned}&\le \delta_{\mathcal{M}}\left\|f\big(H_{U-\mathcal{E}_F(U)}\big)-f\big(H_{V-\mathcal{E}_F(U)}\big)\right\|_1\\ &\le 2\,\big(1-\frac{d}{4}\big)^{-3}\delta_{\mathcal{M}}\,\boldsymbol{L}_{1,\rho_{\widetilde{\mathcal{M}}}}\,\|\mathbb{1}\|^2_{\mathcal{B}\left(W^{1,2}_\Gamma,L^4\right)}\,\overline{m}\,\big\|(H_0+1)^{-1}\big\|_2^2\,\|U-V\|_{L^2},\end{aligned}$$

where the last estimate follows from Lemma 4.1. □

5. The particle density operator

This section is devoted to Lipschitz properties and C^α and $W^{1,p}_\Gamma$ estimates of the particle density operators $\mathcal{N}_\varsigma$. We will use these results later for the existence proof. 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 [35, 36].

5.a. Representation theorem.

5.1. Theorem. *Let U be from $L^2(\Omega)$. Then for any $W\in L^\infty(\Omega)$ the duality between $\tilde{\mathcal{N}}(U)\in L^1(\Omega)$ (cf. Definition 2.16) and W can be written as*

$$\langle\tilde{\mathcal{N}}(U),W\rangle=\int_\Omega\tilde{\mathcal{N}}(U)(x)W(x)\,dx\;=\;\operatorname{tr}\left[f(H_U)W\right]. \tag{5.1}$$

5.2. Remark. 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 2.16), then

$$\langle\mathcal{N}(V),W\rangle=\int_\Omega\tilde{\mathcal{N}}(V-\mathcal{E}_F(V))(x)W(x)\,dx\;=\;\operatorname{tr}\left[f(H_{V-\mathcal{E}_F(V)})W\right]. \tag{5.2}$$

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

In the sequel, we wish to express the norms in several function spaces X by the dual pairing of these spaces with L^∞, because we want to avoid complicated procedures of extending (5.1) to W's from distribution spaces. So we regard test functions from the set

$$K=\{W\in X^*\cap L^\infty,\|W\|_{X^*}=1\}. \tag{5.3}$$

5.3. Lemma. *Suppose $V\in L^2(\Omega)$, $\rho\le\rho_V|_{p=2}$, (cf. (3.6) with $p=2$), $\tilde\rho=-\bar\epsilon_2+2\rho+1-\frac{d}{4}$, (cf. Proposition 4.2), and f and k in accordance with Assumption 2.14. There is*

$$\big\|f(H_V-\mathcal{E}_F(V))(H_V-\rho)^k\big\|\le\boldsymbol{\Lambda}_{k,\tilde\rho}. \tag{5.4}$$

If additionally $\boldsymbol{\Lambda}_{k+1,\tilde\rho}$ is finite, then one has for any $q\ge 1$ with $q>\frac{d}{2}$

$$\left\|f\big(H_V-\mathcal{E}_F(V)\big)(H_V-\rho)^k\right\|_q\le\boldsymbol{\Lambda}_{k+1,\tilde\rho}\big(1-\frac{d}{4}\big)^{-1}\big\|(H_0+1)^{-1}\big\|_q. \tag{5.5}$$

Proof. By Proposition 3.3 item *iii)* the spectrum of $(H_V-\rho)$ is contained in $\left[\frac{1}{4},\infty\right[$. From the spectral theorem — applied to $(H_V-\rho)$, (4.5), and the monotonicity of f, follows

$$\left\|f\big(H_V-\mathcal{E}_F(V)\big)(H_V-\rho)^k\right\| \le \sup_{s\in\left[\frac14,\infty\right[} f(s-\mathcal{E}_F(V)+\rho)s^k$$

$$\le \sup_{s\in\left[\frac14,\infty\right[} f\big(s-\bar\epsilon_2+2\rho+1-\frac{d}{4}\big)s^k = \mathbf{\Lambda}_{k,\tilde\rho}.$$

(5.5) follows now by decomposing

$$\left\|f\big(H_V-\mathcal{E}_F(V)\big)(H_V-\rho)^k\right\|_q = \left\|f\big(H_V-\mathcal{E}_F(V)\big)(H_V-\rho)^{k+1}\right\| \left\|(H_V-\rho)^{-1}\right\|_q$$

and observing (3.8). □

5.4. Remark. One can prove even more easily than Lemma 5.3

$$\left\|f(H_V)(H_V-\rho)^k\right\| \le \mathbf{\Lambda}_{k,\rho} \tag{5.6}$$

and for any $q\ge 1$ with $q>\frac{d}{2}$

$$\left\|f(H_V)(H_V-\rho)^k\right\|_q \le \mathbf{\Lambda}_{k+1,\rho}\big(1-\frac{d}{4}\big)^{-1}\left\|(H_0+1)^{-1}\right\|_q. \tag{5.7}$$

5.5. Lemma. *Let X be a normed space of functions over Ω, which embeds injectively, continuously and densely into $L^1(\Omega)$. Moreover, the image of L^∞ under the adjoint embedding $L^\infty\hookrightarrow X^*$ shall be dense in X^*. Further assume that the duality $\langle\cdot,\cdot\rangle$ between X and its dual space X^* extends the canonical (L^1,L^∞)–duality. Then*

$$\|\tilde{\mathcal{N}}(U)\|_X = \sup_{W\in K}\left|\langle\tilde{\mathcal{N}}(U),W\rangle\right| = \sup_{W\in K}\left|\mathrm{tr}[f(H_U)W)]\right|,\quad U\in L^2(\Omega) \tag{5.8}$$

and

$$\|\tilde{\mathcal{N}}(U)-\tilde{\mathcal{N}}(V)\|_X = \sup_{W\in K}\left|\mathrm{tr}\big[\big(f(H_U)-f(H_V)\big)W\big]\right|,\quad U,V\in L^2(\Omega). \tag{5.9}$$

If $U=V-\mathcal{E}_F(V)$, $\rho\le\rho_V|_{p=2}$ (cf. (3.6) *with $p=2$), $\tilde\rho=-\bar\epsilon_2+2\rho+1-\frac{d}{4}$, (cf. Proposition 4.2), and k is according to Assumption 2.14, then* (5.8) *implies the following estimate of the particle density operator* (2.9)*:*

$$\|\mathcal{N}(V)\|_X = \|\tilde{\mathcal{N}}(V-\mathcal{E}_F(V))\|_X \le \mathbf{\Lambda}_{k,\tilde\rho}\sup_{W\in K}\|(H_V-\rho)^{-k+1}W(H_V-\rho)^{-1}\|_1. \tag{5.10}$$

5.6. Remark. Let be X a normed space and assume

$$\|h\|_X = \sup_{W\in K}|\langle h,W\rangle|\quad\text{for all } h\in X. \tag{5.11}$$

If one additionally already knows that $\tilde{\mathcal{N}}(U),\tilde{\mathcal{N}}(V)$ are from X, then (5.8), (5.10) and (5.9) also hold.

Proof of Lemma 5.5. (5.8) and (5.9) follow from the Hahn–Banach principle, elementary density condiderations and Theorem 5.1. As for (5.10) we estimate

$$\begin{aligned}\|\mathcal{N}(V)\|_X &= \|\tilde{\mathcal{N}}(V-\mathcal{E}_F(V))\|_X = \sup_{W\in K}\left|\mathrm{tr}\left[f\big(H_V-\mathcal{E}_F(V)\big)W\big)\right]\right| \\ &= \sup_{W\in K}\left|\mathrm{tr}\left[f\big(H_V-\mathcal{E}_F(V)\big)(H_V-\rho)^k(H_V-\rho)^{-k+1}W(H_V-\rho)^{-1}\right|\right. \\ &\le \left\|f\big(H_V-\mathcal{E}_F(V)\big)(H_V-\rho)^k\right\|\sup_{W\in K}\left\|(H_V-\rho)^{-k+1}W(H_V-\rho)^{-1}\right\|_1,\end{aligned} \tag{5.12}$$

observing the commutativity of functions of H_V and the commutativity under the trace. Now (5.10) follows with the help of (5.4). $\square$

To obtain optimal results for the one– and two–dimensional case, one has to work with fractional powers of the operator $(H_0+1)^{-1}$. This in mind, we prove

5.7. Lemma. *Assume $d=1$ or $d=2$ and $p>2$ chosen such that* $\mathrm{dom}(H_0)$ *continuously embeds into $W^{1,p}_\Gamma$ (cf. Theorem 2.4 and Remark 2.5). We abbreviate $H_1 = H_0+1$.*

i) *For any $\frac{1}{2}<\alpha<1$ the domain of H_1^α continuously embeds into a space $W^{1,q}_\Gamma$ with $q>2$, namely*

$$\mathrm{dom}(H_1^\alpha)\hookrightarrow W^{1,q}_\Gamma, \qquad \frac{1}{q}=1-\alpha+\frac{2\alpha-1}{p}<\frac{1}{2}. \tag{5.13}$$

Hence,

$$\|H_1^{-\alpha}\|_{\mathcal{B}(W^{-1,q'}_\Gamma,L^2)}=\|H_1^{-\alpha}\|_{\mathcal{B}(L^2,W^{1,q}_\Gamma)}<\infty, \qquad \frac{1}{q'}=1-\frac{1}{q} \tag{5.14}$$

and a fortiori

$$\|H_1^{-\alpha}\|_{\mathcal{B}(L^1,L^2)}=\|H_1^{-\alpha}\|_{\mathcal{B}(L^2,L^\infty)}<\infty. \tag{5.15}$$

ii) *There is*

$$\|H_1^{-\frac{1}{3}}\|_{\mathcal{B}(L^{\frac{4}{3}},L^2)}=H_1^{-\frac{1}{3}}\|_{\mathcal{B}(L^2,L^4)}<\infty. \tag{5.16}$$

iii) *For any $W\in L^2(\Omega)$ (identified with the corresponding multiplication operator) the operator $H_1^{-\frac{2}{3}}WH_1^{-\frac{2}{3}}$ is bounded on $L^2(\Omega)$ and one has*

$$\|H_1^{-\frac{2}{3}}WH_1^{-\frac{2}{3}}\|\le\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^1,L^2)}\|W\|_{L^1}\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,L^\infty)} = \|W\|_{L^1}\|H_1^{-\frac{2}{3}}\|^2_{\mathcal{B}(L^2,L^\infty)}, \tag{5.17}$$

$$\|H_1^{-\frac{2}{3}}WH_1^{-\frac{2}{3}}\|\le 2\|W\|_{W^{-1,q'}_\Gamma}\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,L^\infty)}\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,W^{1,q}_\Gamma)}, \tag{5.18}$$

$$q\in\left[2,\frac{3p}{p+1}\right], \quad \frac{1}{q}+\frac{1}{q'}=1.$$

We will focus our attention to the case $d=2$. The proof for the one–dimensional case runs along the same lines.

Proof of i). Specifying in Theorem 2.29 $\delta=\frac{1}{2}$, $\beta=1$ and $\Theta=2\alpha-1$, one obtains

$$\left[\mathrm{dom}(H_1^{\frac{1}{2}}),\mathrm{dom}(H_1)\right]_{2\alpha-1}=\mathrm{dom}(H_1^\alpha). \tag{5.19}$$

From Definition 2.12 follows that $W^{1,2}_\Gamma$ is the form domain of H_1. The second representation theorem for forms (cf. Kato [28, ch. VI, §2]) states that the form domain is identical with the domain of $H_1^{\frac{1}{2}}$. The premise on p implies that $\mathrm{dom}(H_1)$ continuously embeds into $W^{1,p}_\Gamma$, consequently, $\mathrm{dom}(H_1^\alpha)=\left[W^{1,2}_\Gamma,\mathrm{dom}(H_1)\right]_{2\alpha-1}$ continuously embeds into $\left[W^{1,2}_\Gamma,W^{1,p}_\Gamma\right]_{2\alpha-1}$. This space continuously embeds into $W^{1,q}_\Gamma$ with $\frac{1}{q}=1-\alpha+\frac{2\alpha-1}{p}$. Indeed, its elements satisfy the correct boundary condition because of $\left[W^{1,2}_\Gamma,W^{1,p}_\Gamma\right]_{2\alpha-1}\hookrightarrow W^{1,2}_\Gamma$ and according to Theorem 2.30 there is

$$\left[W^{1,2}_\Gamma,W^{1,p}_\Gamma\right]_{2\alpha-1}\hookrightarrow\left[W^{1,2},W^{1,p}\right]_{2\alpha-1}=W^{1,q}, \quad \frac{1}{q}=1-\alpha+\frac{2\alpha-1}{p}.$$

As $H_1^{-\alpha}$ is selfadjoint on $L^2(\Omega)$, both the terms in (5.15) and (5.14), respectively, are equal. The finiteness of the norms follows from (5.13) and Sobolev's embedding theorem. □

Proof of ii). Again the equality of the norms is a consequence of the selfadjointness of $H_1^{-\alpha}$. Obviously (5.16) is true if $\mathrm{dom}(H_1^{\frac{1}{3}})$ continuously embeds into $L^4(\Omega)$, what we will show now: the interpolation formula for fractional powers (2.28) says that

$$\left[\mathrm{dom}(H_1^0), \mathrm{dom}(H_1^{\frac{1}{2}})\right]_{\frac{2}{3}} = \mathrm{dom}(H_1^{\frac{1}{3}}).$$

As already mentioned above, $\mathrm{dom}(H_1^{\frac{1}{2}})$ is equal to $W_\Gamma^{1,2}$ and, hence, continuously embeds into L^8. Consequently, $\mathrm{dom}(H_1^{\frac{1}{3}})$ continuously embeds into $[L^2, L^8]_{\frac{2}{3}} = L^4$. □

Proof of iii). Now we will prove (5.18), while (5.17) is obviously implied by (5.15). It suffices to prove (5.18) only for functions $W \in W_\Gamma^{-1,q'} \cap L^\infty$ because this space is dense in $W_\Gamma^{-1,q'}$ and the inequality then extends by continuity to the whole space. As $H_1^{-\frac{2}{3}}$ is selfadjoint, there is

$$(5.20)\qquad \begin{aligned} \|H_1^{-\frac{2}{3}} W H_1^{-\frac{2}{3}}\| &= \sup_{\|\psi\|_{L^2}=\|\tilde{\psi}\|_{L^2}=1} \left|\left\langle H_1^{-\frac{2}{3}} W H_1^{-\frac{2}{3}}\psi, \tilde{\psi}\right\rangle\right| \\ &= \sup_{\|\psi\|_{L^2}=\|\tilde{\psi}\|_{L^2}=1} \left|\left\langle W H_1^{-\frac{2}{3}}\psi, H_1^{-\frac{2}{3}}\tilde{\psi}\right\rangle\right| \end{aligned}$$

The duality between $W_\Gamma^{1,q}$ and $W_\Gamma^{-1,q'}$ is the extended (L^1, L^∞)–duality, hence,

$$(5.21)\qquad \begin{aligned} \left|\left\langle W H_1^{-\frac{2}{3}}\psi, H_1^{-\frac{2}{3}}\tilde{\psi}\right\rangle\right| &\le \|W\|_{W_\Gamma^{-1,q'}} \left\|\left(H_1^{-\frac{2}{3}}\psi\right)\left(H_1^{-\frac{2}{3}}\tilde{\psi}\right)^*\right\|_{W_\Gamma^{1,q}} \\ &\le \|W\|_{W_\Gamma^{-1,q'}} \left(\left\|H_1^{-\frac{2}{3}}\psi\right\|_{L^\infty}\left\|H_1^{-\frac{2}{3}}\tilde{\psi}\right\|_{W_\Gamma^{1,q}} + \left\|H_1^{-\frac{2}{3}}\psi\right\|_{W_\Gamma^{1,q}}\left\|H_1^{-\frac{2}{3}}\tilde{\psi}\right\|_{L^\infty}\right) \\ &\le 2\,\|W\|_{W_\Gamma^{-1,q'}} \|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,L^\infty)} \|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,W_\Gamma^{1,q})} \|\tilde{\psi}\|_{L^2}\|\psi\|_{L^2}. \end{aligned}$$

According to (5.15), $\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,W_\Gamma^{1,\frac{3p}{p+1}})}$ is finite, the more is $\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,W_\Gamma^{1,q})}$ for $q \in \left[2, \frac{3p}{p+1}\right[$. This, together with (5.20) and (5.21), proves (5.18). □

5.b. **A priori estimates.** Now we will derive estimates of the carrier density operators. We have to distinguish the cases $d = 1$, $d = 2$ and $d = 3$, because on the one hand the resolvents $(H_0 + 1)^{-1}$ of the Hamiltonian differ in their mapping and summability properties, depending on d, and on the other hand the C^α–bounds in the case $d = 3$ cannot be achieved with the help of Lemma 5.5. We have decided to present all proofs in detail, because the knowledge on the norm boundedness of the carrier densities in function spaces compactly embedding into L^1 is essential for the existence proof later on. Furthermore, the C^α estimates, which follow in all dimensions $d = 1, 2, 3$ from the presented results, are in our context the only instrument to control the oscillation behaviour of the carrier densities.

5.8. Proposition. *The operator $V \longmapsto \mathcal{N}(V) = \tilde{\mathcal{N}}(V - \mathcal{E}_F(V))$, where $\mathcal{N}$ is the carrier density operator from Definition 2.16, is well defined as an operator from $L^2(\Omega)$ into $L^1(\Omega)$. Let $\mathcal{M}$ be a bounded set in $L^2(\Omega)$, d the dimension of the spatial domain Ω, $\rho \le \rho_{\mathcal{M}}$ as in (3.22), $\tilde{\rho} = -\bar{\epsilon}_2 + 2\rho + 1 - \frac{d}{4}$, (cf. Proposition 4.2), and $\mathbf{\Lambda}_{k,\tilde{\rho}}$ according to (2.5). We abbreviate again $H_1 = H_0 + 1$.*

i) $d=1$: *Let* $\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}$ *denote the embedding constant from* $W^{1,2}_\Gamma$ *into* L^∞, *which is finite for* $d=1$. *The particle density operator* $\mathcal{N}$ *takes its values in* $W^{1,2}_\Gamma(\Omega)$ *and*

$$\sup_{V\in\mathcal{M}}\|\mathcal{N}(V)\|_{W^{1,2}_\Gamma}\le 4\,\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\boldsymbol{\Lambda}_{2,\tilde\rho}\|H_1^{-1}\|_1. \tag{5.22}$$

ii) $d=1$ *or* $d=2$: *If* $\|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}_\Gamma)}$ *is finite for some* $p\ge 2$, *then* $\mathcal{N}$ *takes its values in* $W_\Gamma^{1,\frac{3p}{p+1}}$ *and*

$$\begin{aligned}\sup_{V\in\mathcal{M}}\big\|\mathcal{N}(V)\big\|_{W_\Gamma^{1,\frac{3p}{p+1}}}\le 2\big(1-\frac{d}{4}\big)^{-1}\boldsymbol{\Lambda}_{3,\tilde\rho}\big\|H_1^{-1}\big\|_2\big\|H_1^{-\frac{2}{3}}\big\|_2\\ \cdot\big\|H_1^{-\frac{2}{3}}\big\|_{\mathcal{B}(L^2,L^\infty)}\big\|H_1^{-\frac{2}{3}}\big\|_{\mathcal{B}(L^2,W_\Gamma^{1,\frac{3p}{p+1}})}\sup_{V\in\mathcal{M}}\big\|H_1(H_V-\rho)^{-1}\big\|^2.\end{aligned} \tag{5.23}$$

iii) $d=3$: *If* $\|H_1^{-1}\|_{\mathcal{B}(L^2,C^\alpha)}$ *is finite, then* $\mathcal{N}$ *takes its values in* C^α *and if* $\|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}_\Gamma)}$ *is finite, then its values are contained in* $W^{1,p}_\Gamma$. *Moreover,*

$$\begin{aligned}\sup_{V\in\mathcal{M}}\big\|\mathcal{N}(V)\big\|_{L^\infty}&\le\sup_{V\in\mathcal{M}}\big\|\mathcal{N}(V)\big\|_{C^\alpha}\\ &\le 16\,\boldsymbol{\Lambda}_{4,\tilde\rho}\big\|H_1^{-1}\big\|^2_{\mathcal{B}(L^2,C^\alpha)}\big\|H_1^{-1}\big\|^2_2\sup_{V\in\mathcal{M}}\big\|H_1(H_V-\rho)^{-1}\big\|^2\end{aligned} \tag{5.24}$$

$$\begin{aligned}\sup_{V\in\mathcal{M}}\big\|\mathcal{N}(V)\big\|_{W^{1,p}_\Gamma}\le 32\,\boldsymbol{\Lambda}_{4,\tilde\rho}\big\|H_1^{-1}\big\|_{\mathcal{B}(L^2,L^\infty)}\big\|H_1^{-1}\big\|_{\mathcal{B}(L^2,W^{1,p}_\Gamma)}\big\|H_1^{-1}\big\|_2^2\\ \cdot\sup_{V\in\mathcal{M}}\big\|H_1(H_V-\rho)^{-1}\big\|^2.\end{aligned} \tag{5.25}$$

The assertion that $\mathcal{N}:L^2(\Omega)\to L^1(\Omega)$ is well defined follows from the estimates stated in Proposition 5.8.

Proof of i). According to Definition 2.16 one has for any $V\in\mathcal{M}$

$$\|\mathcal{N}(V)\|_{W^{1,2}_\Gamma}\le\sum_{l=1}^\infty f(\mathcal{E}_l(V)-\mathcal{E}_F(V))\big\||\psi_l(V)|^2\big\|_{W^{1,2}_\Gamma}.$$

Observing (3.7) and (3.27), we estimate

$$\begin{aligned}\big\||\psi_l(V)|^2\big\|_{W^{1,2}_\Gamma}&\le 2\|\psi_l(V)\|_{L^\infty}\|\psi_l(V)\|_{W^{1,2}_\Gamma}\\ &\le 2\big\|H_1^{-\frac12}\big\|_{\mathcal{B}(L^2,L^\infty)}\big\|H_1^{\frac12}\psi_l(V)\big\|_{L^2}\big\|H_1^{-\frac12}\big\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)}\|H_1^{\frac12}\psi_l(V)\|_{L^2}\\ &\le 2\big\|H_1^{-\frac12}\big\|_{\mathcal{B}(L^2,L^\infty)}\big\|H_1^{-\frac12}\big\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)}\big\|H_1^{\frac12}(H_V-\rho)^{-\frac12}\big\|^2\big\|(H_V-\rho)^{\frac12}\psi_l(V)\big\|^2_{L^2}\\ &\le 2\,\big\|H_1^{-\frac12}\big\|_{\mathcal{B}(L^2,L^\infty)}\big\|H_1^{-\frac12}\big\|_{\mathcal{B}(L^2,W^{1,2}_\Gamma)}\big(1-\frac{d}{4}\big)^{-1}(\mathcal{E}_l(V)-\rho)\\ &\le 2\,\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\,(1-\frac{d}{4})^{-1}(\mathcal{E}_l(V)-\rho).\end{aligned}$$

Hence,

$$\begin{aligned}\big\|\mathcal{N}(V)\big\|_{W^{1,2}_\Gamma}&\le 2\,\big(1-\frac{d}{4}\big)^{-1}\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\sum_{l=1}^\infty f(\mathcal{E}_l(V)-\mathcal{E}_F(V))(\mathcal{E}_l(V)-\rho)\\ &=2\,\big(1-\frac{d}{4}\big)^{-1}\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_\Gamma,L^\infty)}\overline{m}\,\big\|f(H_V-\mathcal{E}_F(V))(H_V-\rho)\big\|_1.\end{aligned}$$

One arrives now at (5.22) with the help of (5.5). □

Proof of ii). In this part of the proof we abbreviate $X = W_\Gamma^{1,\frac{3p}{p+1}}$, hence, $X^* = W_\Gamma^{-1,\frac{3p}{2p-1}}$. K denotes again the set (5.3). According to Lemma 5.5, (5.10) there is for any $V \in \mathcal{M}$

$$\begin{aligned}
\|\mathcal{N}(V)\|_X &\le \sup_{W \in K} \mathbf{\Lambda}_{3,\tilde{\rho}} \left\|(H_V-\rho)^{-2} W (H_V-\rho)^{-1}\right\|_1 \\
&\le \mathbf{\Lambda}_{3,\tilde{\rho}} \left\|(H_V-\rho)^{-1}\right\|_2 \sup_{W \in K} \left\|(H_V-\rho)^{-1} W (H_V-\rho)^{-1}\right\|_2 \\
&\le \mathbf{\Lambda}_{3,\tilde{\rho}} \big(1-\frac{d}{4}\big)^{-1} \|H_1^{-1}\|_2 \|H_1 (H_V-\rho)^{-1}\|^2 \sup_{W \in K} \|H_1^{-1} W H_1^{-1}\|_2,
\end{aligned}$$

N.B. (3.8). Now one estimates

$$\begin{aligned}
\sup_{W \in K} \|H_1^{-1} W H_1^{-1}\|_2 &\le \left\|H_1^{-\frac{1}{3}}\right\|_4^2 \sup_{W \in K} \left\|H_1^{-\frac{2}{3}} W H_1^{-\frac{2}{3}}\right\| \\
&\le 2 \left\|H_1^{-\frac{2}{3}}\right\|_2 \left\|H_1^{-\frac{2}{3}}\right\|_{\mathcal{B}(L^2,L^\infty)} \left\|H_1^{-\frac{2}{3}}\right\|_{\mathcal{B}(L^2,X)},
\end{aligned}$$

thereby using Lemma 5.7, (5.18) and Theorem 2.27, (2.26). □

Proof of iii). First we prove (5.25). According to Definition 2.16 one has for any $V \in \mathcal{M}$

$$\|\mathcal{N}(V)\|_{W_\Gamma^{1,p}} \le \sum_{l=1}^\infty f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) \left\| |\psi_l(V)|^2 \right\|_{W_\Gamma^{1,p}}. \tag{5.26}$$

We estimate the items separately

$$\begin{aligned}
\left\| |\psi_l(V)|^2 \right\|_{W_\Gamma^{1,p}} &\le 2 \|\psi_l(V)\|_{L^\infty} \|\psi_l(V)\|_{W_\Gamma^{1,p}} \\
&\le 2 \|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)} \|H_1^{-1}\|_{\mathcal{B}(L^2,W_\Gamma^{1,p})} \|H_1 \psi_l(V)\|_{L^2}^2
\end{aligned}$$

and therein

$$\begin{aligned}
\|H_1 \psi_l(V)\|_{L^2} &\le \|(H_V-\rho)\psi_l(V)\|_{L^2} \sup_{V \in \mathcal{M}} \|H_1 (H_V-\rho)^{-1}\| \\
&= \big(\mathcal{E}_l(V) - \rho\big) \sup_{V \in \mathcal{M}} \|H_1 (H_V-\rho)^{-1}\|.
\end{aligned}$$

We now continue (5.26)

$$\begin{aligned}
\|\mathcal{N}(V)\|_{W_\Gamma^{1,p}} &\le 2 \|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)} \|H_1^{-1}\|_{\mathcal{B}(L^2,W_\Gamma^{1,p})} \\
&\quad \cdot \sup_{V \in \mathcal{M}} \|H_1 (H_V-\rho)^{-1}\|^2 \sum_{l=1}^\infty f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) (\mathcal{E}_l(V) - \rho)^2
\end{aligned}$$

and estimate

$$\begin{aligned}
\sum_{l=1}^\infty f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) (\mathcal{E}_l(V) - \rho)^2 &= \|f(H_V - \mathcal{E}_F(V))(H_V-\rho)^2\|_1 \\
&\le \|f(H_V - \mathcal{E}_F(V))(H_V-\rho)^4\| \, \|(H_V-\rho)^{-1}\|_2^2 \\
&\le \mathbf{\Lambda}_{4,\tilde{\rho}} \big(1-\frac{d}{2p}\big)^{-2} \|H_1^{-1}\|_2^2 \le 16\, \mathbf{\Lambda}_{4,\tilde{\rho}} \|H_1^{-1}\|_2^2
\end{aligned}$$

with the help of (5.4) and (3.8), which finishes the proof of (5.25).

In order to prove (5.24), one uses the inequality

$$\left\| |\psi_l(V)|^2 \right\|_{C^\alpha} \le \|\psi_l(V)\|_{C^\alpha}^2 \le \|H_1^{-1}\|_{\mathcal{B}(L^2,C^\alpha)}^2 \|H_1 \psi_l(V)\|_{L^2}^2$$

to estimate the terms in

$$\|\mathcal{N}(V)\|_{C^\alpha} \leq \sum_{l=1}^{\infty} f(\mathcal{E}_l(V) - \mathcal{E}_F(V)) \big\| |\psi_l(V)|^2 \big\|_{C^\alpha}.$$

The remaining part of the proof for (5.24) is as before. □

5.9. Corollary. *Proposition 5.8 implies L^∞–estimates in all dimensions $d = 1, 2, 3$. Thus in connection with* (2.10) *one obtains L^p–bounds for the values of the particle density operators:*

$$\sup_{V \in \mathcal{M}} \|\mathcal{N}(V)\|_{L^p(\Omega)} \leq N^{\frac{1}{p}} \sup_{V \in \mathcal{M}} \|\mathcal{N}(V)\|_{L^\infty(\Omega)}^{\frac{p-1}{p}}. \tag{5.27}$$

We can also give $W_\Gamma^{-1,2}$–estimates for the particle density operators.

5.10. Proposition. *We abbreviate again $H_1 = H_0 + 1$ and regard the particle density operator $\mathcal{N}$ from Definition 2.16.*

i) *If $d = 1$ then for any $V \in L^2(\Omega)$*

$$\|\mathcal{N}(V)\|_{W_\Gamma^{-1,2}} \leq N \, \|\mathbb{1}\|_{\mathcal{B}(L^1, W_\Gamma^{-1,2})}, \tag{5.28}$$

where N is the total amount of the particle species under consideration, cf. Definition 2.16.

ii) *If $d = 2$ or $d = 3$, $\mathcal{M}$ is a $L^2(\Omega)$-bounded set, $V \in \mathcal{M}$, ρ is in accordance with* (3.22), *and $\tilde{\rho} = -\bar{\epsilon}_2 + 2\rho + 1 - \frac{d}{4}$, (cf. Proposition 4.2), then*

$$\|\mathcal{N}(V)\|_{W_\Gamma^{-1,2}} \leq \mathbf{\Lambda}_{2,\tilde{\rho}} \left(1 - \frac{d}{4}\right)^{-2} \|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2}, L^6)} \|H_1^{-\frac{1}{4}}\|_{\mathcal{B}(L^2, L^3)} \|H_1^{-\frac{7}{4}}\|_1 < \infty. \tag{5.29}$$

Proof. (5.28) follows easily by embedding $L^1 \hookrightarrow W_\Gamma^{-1,2}$ and from the L^1–normalization condition (2.10) for $\mathcal{N}$.

Now let K be the intersection of $L^\infty(\Omega)$ with the unit ball of $W_\Gamma^{1,2}(\Omega)$. Observing the commutativity implied by the spectral theorem and the commutativity under the trace one obtains by means of Theorem 5.1

$$\begin{aligned}
\|\mathcal{N}(V)\|_{W_\Gamma^{-1,2}} &= \sup_{W \in K} \big|\langle \mathcal{N}(V), W \rangle\big| = \sup_{W \in K} \Big|\mathrm{tr}\big[f(H_V - \mathcal{E}_F(V)) W\big]\Big| \\
&= \sup_{W \in K} \Big|\mathrm{tr}\big[f(H_V - \mathcal{E}_F(V))\,(H_V - \rho)\,(H_V - \rho)^{-\frac{1}{2}} W \,(H_V - \rho)^{-\frac{1}{2}}\big]\Big| \\
&\leq \sup_{W \in K} \big\|f(H_V - \mathcal{E}_F(V))\,(H_V - \rho)\big\|_{\frac{7}{4}} \big\|(H_V - \rho)^{-\frac{1}{2}} W \,(H_V - \rho)^{-\frac{1}{2}}\big\|_{\frac{7}{3}}
\end{aligned}$$

Further, Lemma 5.3 and (3.7) imply

$$\begin{aligned}
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}} \big(1 - \frac{1}{4}\big)^{-1} \big\|H_1^{-1}\big\|_{\frac{7}{4}} \sup_{W \in K} \big\|(H_V - \rho)^{-\frac{1}{2}} W \,(H_V - \rho)^{-\frac{1}{2}}\big\|_{\frac{7}{3}} \\
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}} \big(1 - \frac{1}{4}\big)^{-1} \big\|H_1^{-1}\big\|_{\frac{7}{4}} \big\|(H_V - \rho)^{-\frac{1}{2}} H_1^{\frac{1}{2}}\big\|^2 \sup_{W \in K} \big\|H_1^{-\frac{1}{2}} W \, H_1^{-\frac{1}{2}}\big\|_{\frac{7}{3}} \\
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}} \big(1 - \frac{1}{4}\big)^{-2} \big\|H_1^{-1}\big\|_{\frac{7}{4}} \sup_{W \in K} \big\|H_1^{-\frac{1}{2}} W \, H_1^{-\frac{1}{2}}\big\|_{\frac{7}{3}} \\
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}} \big(1 - \frac{1}{4}\big)^{-2} \big\|H_1^{-1}\big\|_{\frac{7}{4}} \big\|H_1^{-\frac{1}{2}}\big\|_{\frac{7}{2}} \big\|H_1^{-\frac{1}{4}}\big\|_{7} \sup_{W \in K} \big\|W \, H_1^{-\frac{1}{4}}\big\|
\end{aligned}$$

According to (2.26), one has $\|H_1^{-1}\|_{\frac{7}{4}}\|H_1^{-\frac{1}{2}}\|_{\frac{7}{2}}\|H_1^{-\frac{1}{4}}\|_7 = \|H_1^{-\frac{7}{4}}\|_1$, which is finite for the spatial dimensions $d = 1, 2, 3$ under consideration (cf. Theorem 2.13), and we continue

$$\begin{aligned}
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}}\big(1-\frac{1}{4}\big)^{-2}\|H_1^{-\frac{7}{4}}\|_1 \sup_{W\in K}\|W\,H_1^{-\frac{1}{4}}\| \\
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}}\big(1-\frac{1}{4}\big)^{-2}\|H_1^{-\frac{7}{4}}\|_1\|H_1^{-\frac{1}{4}}\|_{\mathcal{B}(L^2,L^3)} \sup_{W\in K}\|W\|_{L^6} \\
&\leq \mathbf{\Lambda}_{2,\tilde{\rho}}\big(1-\frac{1}{4}\big)^{-2}\|H_1^{-\frac{7}{4}}\|_1\|H_1^{-\frac{1}{4}}\|_{\mathcal{B}(L^2,L^3)}\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^6)},
\end{aligned}$$

where $\|\mathbb{1}\|_{\mathcal{B}(W_\Gamma^{1,2},L^6)}$ is the embedding constant of $W_\Gamma^{1,2} \hookrightarrow L^6$.

Obviously, $\|H_1^{-\frac{1}{4}}\|_{\mathcal{B}(L^2,L^3)}$ is finite, if $\mathrm{dom}(H_1^{\frac{1}{4}})$ continuously embeds into L^3, what we will show now: the interpolation formula for fractional powers (2.28) says that

$$\Big[\mathrm{dom}(H_1^0, \mathrm{dom}(H_1^{\frac{1}{2}})\Big]_{\frac{1}{2}} = \mathrm{dom}(H_1^{\frac{1}{4}}).$$

As already mentioned, $\mathrm{dom}(H_1^{\frac{1}{2}})$ is equal to $W_\Gamma^{1,2}$, which continuously embeds into L^6. Consequently, $\mathrm{dom}(H_1^{\frac{1}{4}})$ continuously embeds into $[L^2, L^6]_{\frac{1}{2}} = L^3$. □

5.11. Remark. There are also estimates of the pseudo particle density operator $\tilde{\mathcal{N}}$ (cf. Definition 2.16), which are analogous to those in Proposition 5.8, Corollary 5.9, and Proposition 5.10. According to Assumption 2.14, the L^1–norm of $\tilde{\mathcal{N}}(V)$ is bounded

$$\big\|\tilde{\mathcal{N}}(V)\big\|_{L^1} \leq \mathbf{\Lambda}_{0,0}, \qquad \text{for all } V \in L^2(\Omega). \tag{5.30}$$

Moreover, if $\rho \leq \rho_V|_{p=2}$, (cf. (3.6) with $p = 2$), then

$$\big\|f(H_V)(H_V - \rho)^k\big\| \leq \mathbf{\Lambda}_{k,\rho} \tag{5.31}$$

and one has for any $1 \leq q \leq \infty$ with $q > \frac{d}{2}$

$$\big\|f(H_V)(H_V - \rho)^k\big\|_q \leq \mathbf{\Lambda}_{k+1,\rho}\big(1 - \frac{d}{4}\big)^{-1}\big\|(H_0 + 1)^{-1}\big\|_q. \tag{5.32}$$

Hence, the estimates from Proposition 5.8, Corollary 5.9, and Proposition 5.10 are true for $\tilde{\mathcal{N}}$ instead of $\mathcal{N}$, while replacing $\tilde{\rho}$ by ρ and N by $\mathbf{\Lambda}_{0,0}$. In particular this ensures that $\tilde{\mathcal{N}}(V)$ belongs to $C(\overline{\Omega})$ for all $V \in L^2(\Omega)$, and the defining series converges uniformly on $\overline{\Omega}$ towards the density $\tilde{\mathcal{N}}(V)$.

5.c. **Boundary behaviour.** In the next proposition we will deal with the boundary behaviour of the values of the pseudo particle density operator $\tilde{\mathcal{N}}$, 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 there. Moreover, the normal derivative of $\tilde{\mathcal{N}}(V)$ vanishes — in a certain sense — on the whole boundary of Ω. In order to give an adequate formulation of this boundary behaviour, we introduce a trace operator and establish a corresponding Gauss–Green formula.

5.12. Definition. Suppose $\Omega \subset \mathbb{R}^d$ as in Definition 2.2 and $p \in]1, \infty[$. Further, let

$$\mathrm{sp} : W^{1,p}(\Omega) \longmapsto W^{1-\frac{1}{p},p}(\partial\Omega)$$

be the usual trace mapping $\phi \mapsto \mathrm{sp}(\phi)$, which maps a $W^{1,p}$–function ϕ on Ω to the trace $\mathrm{sp}(\phi) = \phi|_{\partial\Omega}$ of this function on the boundary of Ω, cf. [21]. Moreover, we define sp_ν as the mapping

$$\mathrm{sp}_\nu : C^1(\overline{\Omega}, \mathbb{R}^d) \longmapsto L^\infty(\partial\Omega) \hookrightarrow \left(W^{1-\frac{1}{p},p}(\partial\Omega)\right)^*, \qquad \mathrm{sp}_\nu\big((\phi_1, \dots, \phi_d)\big) = \sum_{j=1}^{d} \nu_j \,\mathrm{sp}(\phi_j),$$

where ν is the outer unit normal on the boundary of Ω. Finally we define the space E_p as

$$E_p = \left\{ w : w \in L^{\frac{d}{d-1}}(\Omega, \mathbb{R}^d),\ \operatorname{div} w \in L^p(\Omega) \right\}, \qquad p > 1,$$

topologized by $\| \cdot \|_{L^{\frac{d}{d-1}}(\Omega,\mathbb{R}^d)} + \| \operatorname{div}(\cdot) \|_{L^p(\Omega)}$.

5.13. Lemma. *For any $p \in]1, \infty[$ the space $C^1(\overline{\Omega}, \mathbb{R}^d)$ is dense in E_p.*

Proof. According to the Hahn–Banach theorem it is sufficient to prove that any linear continuous functional over E_p, which vanishes on $C^1(\overline{\Omega}, \mathbb{R}^d)$, is identically zero. First, it is easy to see that any linear continuous functional on E_p has the form

$$w \longmapsto \int_\Omega \phi \operatorname{div} w \, dx \; + \; \int_\Omega \langle w, \tilde{\phi} \rangle \, dx, \qquad \tilde{\phi} \in L^d(\Omega, \mathbb{R}^d), \quad \phi \in L^{\frac{p}{p-1}}(\Omega). \tag{5.33}$$

The argument is the same as in the representation theorem for the elements of $W^{-1,p}(\Omega)$, cf. e.g. [49]. Suppose now that a functional of the form (5.33) vanishes on the subspace $C^1(\overline{\Omega}, \mathbb{R}^d)$ of E_q. Taking test functions w from $C_0^\infty(\Omega, \mathbb{R}^d) \subset C^1(\overline{\Omega}, \mathbb{R}^d)$ with only one nonvanishing component, one deduces from the definition of the partial derivative of a distribution

$$\frac{\partial \phi}{\partial x_j} = \tilde{\phi}_j \in L^d(\Omega), \qquad j = 1, \dots, d.$$

By means of the Gauss–Green formula for $W^{1,p}$–spaces (cf. [21]) now follows

$$\int_{\partial\Omega} \langle \nu, w \rangle \ \mathrm{sp}(\phi) \, d\tau = 0, \qquad \text{for all} \quad w \in C^1(\overline{\Omega}, \mathbb{R}^d), \tag{5.34}$$

where $d\tau$ denotes integration with respect to the surface measure on $\partial\Omega$. Next we conclude that $\mathrm{sp}(\phi)$ vanishes almost everywhere with respect to the surface measure on $\partial\Omega$, which implies $\phi \in W_0^{1,d}(\Omega)$ (cf. [19]). Indeed, regarding (5.34) for functions $w \in C^1(\overline{\Omega}, \mathbb{R}^d)$ with only one nonvanishing component, one gets that for any $j \in \{1, \dots, d\}$ the Radon measure

$$\mu_j : f \longmapsto \int_{\partial\Omega} \nu_j(\tau) f(\tau) sp(\phi)(\tau) \, d\tau$$

vanishes on the subspace $\{\mathrm{sp}(g) : g \in C^1(\overline{\Omega})\}$ of $C(\partial\Omega)$. By the Stone–Weierstraß theorem, this subspace is dense in $C(\partial\Omega)$, hence, all the measures μ_j are identically zero. From this, one easily deduces that all the functions $\nu_j(\cdot)\phi(\cdot)$ must vanish almost everywhere with respect to the surface measure on $\partial\Omega$, what implies that ϕ itself has to vanish almost everywhere on $\partial\Omega$. Now let $w \in E_p$ be arbitrary. Then

$$\phi \longmapsto \int_\Omega \sum_{j=1}^{d} w_j \frac{\partial \phi}{\partial x_j} \, dx \; + \; \int_\Omega \phi \operatorname{div} w \, dx$$

is a linear continuous functional on $W^{1,d}(\Omega)$, which annihilates the subspace $C_0^\infty(\Omega)$. As $C_0^\infty(\Omega)$ is dense in $W_0^{1,d}(\Omega)$, it also annihilates any element from $W_0^{1,d}(\Omega)$. □

5.14. Lemma. *For any $p \in]1,\infty[$ the mapping sp_ν (cf. Definition 5.12) extends uniquely to a mapping from E_p into $\big(W^{1-\frac{1}{d},d}(\partial\Omega)\big)^*$ and one has for all $w \in E_p$ and all $\phi \in W^{1,d}(\Omega)$ the generalized Gauss–Green formula*

$$(5.35)\qquad \int_\Omega \phi \operatorname{div} w \, dx + \int_\Omega \langle w, \operatorname{grad} \phi \rangle_{\mathbb{R}^d} \, dx = \Big\langle \mathrm{sp}_\nu(w), \mathrm{sp}(\phi) \Big\rangle_{\big[\big(W^{1-\frac{1}{d},d}(\partial\Omega)\big)^*, W^{1-\frac{1}{d},d}(\partial\Omega)\big]}.$$

Lemma 5.14 and its proof are similar to [41, Theorem 2.1]. The uniqueness of the extension for the mapping sp_ν to the whole space E_p follows from Lemma 5.13.

5.15. Proposition. *For any $V \in L^2(\Omega)$ the particle density $\tilde{\mathcal{N}}(V)$ (cf. Definition 2.16) has the following trace properties (cf. Definition 5.12) on the boundary of the domain Ω:*

$$(5.36)\qquad \tilde{\mathcal{N}}(V)|_\Gamma = 0, \qquad \textit{as an equation in } C(\Gamma),$$

$$(5.37)\qquad \mathrm{sp}_\nu\big(m^{-1} \operatorname{grad} \tilde{\mathcal{N}}(V)\big) = 0, \qquad \textit{as an equation in } \big(W^{1-\frac{1}{d},d}(\partial\Omega)\big)^*.$$

5.16. Remark. If $d = 1$, then (5.37) a fortiori is true as an equation in $\big(W^{\frac{1}{2},2}(\partial\Omega)\big)^*$, i.e. in the usual sense (cf. [41]).

Proof of (5.36). According to Remark 5.11 the series $\sum_{l=1}^\infty f(\mathcal{E}_l(V))|\psi_l(V)|^2$, defining $\tilde{\mathcal{N}}(V)$, converges in the space $C(\overline{\Omega})$ and the property $\psi_l|_\Gamma = 0$ of the eigenfunctions passes to the density $u = \tilde{\mathcal{N}}(V)$. □

Proof of (5.37). We abbreviate $X = W^{1-\frac{1}{d},d}(\partial\Omega)$ and $H_1 = H_0 + 1$. As the Schrödinger operator H_V from Definition 2.12 is selfadjoint and commutes with the complex conjugation on the underlying Hilbert space one can always find an orthonormal system of real eigenfunctions, and we refer to that in the following. For any (real) eigenfunction ψ_l of H_V there is

$$(5.38)\qquad \big\langle \mathrm{sp}_\nu(m^{-1} \operatorname{grad} \psi_l), \mathrm{sp}(h) \big\rangle_{[X^*,X]} = 0, \qquad \text{for all } h \in W^{1,2}_\Gamma$$

(cf. [19, ch. II \$ 2]). Moreover, the distributions

$$(5.39)\qquad \operatorname{div}\big(m^{-1} \operatorname{grad} \psi_l^2\big) = 2\,\psi_l H_0 \psi_l + 2\,\big\langle \operatorname{grad} \psi_l, m^{-1} \operatorname{grad} \psi_l \big\rangle_{\mathbb{R}^d}$$

are from a space $L^q(\Omega)$ with $q > 1$. Indeed, observing Proposition 3.7 and Corollary 2.7, one can estimate the items in (5.39) as follows:

$$(5.40)\qquad \begin{aligned} \|\psi_l\|_{L^\infty} &\le \|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)} \|H_1 \psi_l\|_{L^2} \\ &\le \|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)} \|H_1 (H_V - \rho)^{-1}\|_{\mathcal{B}(L^2,L^2)} \|(H_V - \rho)\psi_l\|_{L^2} \\ &= \|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)} \|H_1 (H_V - \rho)^{-1}\|_{\mathcal{B}(L^2,L^2)} \big(\mathcal{E}_l(V) - \rho\big) < \infty \end{aligned}$$

and

$$(5.41)\qquad \begin{aligned} \|\psi_l\|_{W^{1,p}} &\le \|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p})} \|H_1 \psi_l\|_{L^2} \\ &\le \|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}} \|H_1 (H_V - \rho)^{-1}\|_{\mathcal{B}(L^2,L^2)} \|(H_V - \rho)\psi_l\|_{L^2} \\ &= \|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}} \|H_1 (H_V - \rho)^{-1}\|_{\mathcal{B}(L^2,L^2)} \big(\mathcal{E}_l(V) - \rho\big) < \infty, \end{aligned}$$

where ρ is well beyond the spectrum of H_V (cf. Corollary 3.7), and $p > 2$ such that $\|(H_0 + 1)^{-1}\|_{\mathcal{B}(L^2,W^{1,p})}$ is finite, cf. Theorem 2.4 and Remark 2.5.

Thus $\psi_l^2 \in E_q$, for some $q > 1$. Hence, the generalized Gauss–Green formula (5.35) provides for any $h \in W^{1,d}(\Omega)$

$$
\begin{aligned}
(5.42)\quad & \big\langle \mathrm{sp}_\nu(m^{-1}\,\mathrm{grad}\,\psi_l^2), \mathrm{sp}(h)\big\rangle_{[X^*,X]} \\
&= \int_\Omega h\,\mathrm{div}(m^{-1}\,\mathrm{grad}\,\psi_l^2)\,dx + \int_\Omega \langle m^{-1}\,\mathrm{grad}\,\psi_l^2, \mathrm{grad}\,h\rangle_{\mathbb{R}^d}\,dx \\
&= 2\left[\int_\Omega h\,\mathrm{div}(\psi_l\, m^{-1}\,\mathrm{grad}\,\psi_l)\,dx + \int_\Omega \langle \psi_l\, m^{-1}\,\mathrm{grad}\,\psi_l, \mathrm{grad}\,h\rangle_{\mathbb{R}^d}\,dx\right] \\
&= 2\Bigg[\int_\Omega h\,\langle m^{-1}\,\mathrm{grad}\,\psi_l, \mathrm{grad}\,\psi_l\rangle_{\mathbb{R}^d}\,dx + \int_\Omega \psi_l\, h\,\mathrm{div}(m^{-1}\,\mathrm{grad}\,\psi_l)\,dx \\
&\quad + \int_\Omega \langle m^{-1}\,\mathrm{grad}\,\psi_l, \mathrm{grad}(\psi_l\, h)\rangle_{\mathbb{R}^d}\,dx - \int_\Omega h\,\langle m^{-1}\,\mathrm{grad}\,\psi_l, \mathrm{grad}\,\psi_l\rangle_{\mathbb{R}^d}\,dx\Bigg] \\
&= 2\big\langle \mathrm{sp}_\nu(m^{-1}\,\mathrm{grad}\,\psi_l), \mathrm{sp}(\psi_l\, h)\big\rangle_{[X^*,X]}
\end{aligned}
$$

From (5.38) follows that the last term is zero, because $h \in W^{1,d}(\Omega)$ and $\psi_l \in W_\Gamma^{1,p}(\Omega)$, $(p > 2)$ imply $\psi_l h \in W_\Gamma^{1,2}(\Omega)$. Taking into account (5.40), (5.41), (5.42) and the decay properties of the sequence $\{f(\mathcal{E}_l(V))\}$ (cf. Assumption 2.14), one easily verifies that the series

$$
\sum_l f(\mathcal{E}_l(V)) sp_\nu(m^{-1}\,\mathrm{grad}\,\psi_l^2)
$$

converges in $\big(W^{1-\frac{1}{d},d}(\partial\Omega)\big)^*$, what proves (5.37). □

5.d. **Lipschitz continuity.** The next statements are concerned with the Lipschitz properties of the mapping $\tilde{\mathcal{N}}$, regarded from $L^2(\Omega)$ into several target spaces. Some of the results are needed explicitely in our later considerations, some are stated, because the authors believe that they are interesting in themselves. The proofs are based on the representation Theorem 5.1 and the Birman–Solomjak Theorem 2.28. We start with the simplest case, the —natural— target space L^1 for the carrier density operators.

5.17. Proposition. *The (pseudo) carrier density operators $\tilde{\mathcal{N}} : L^2 \longmapsto L^1$ are locally Lipschitz continuous:*

$$
\big\|\tilde{\mathcal{N}}(U) - \tilde{\mathcal{N}}(V)\big\|_{L^1} \le 2\left(1 - \frac{d}{4}\right)^{-3} \boldsymbol{L}_{1,\rho_\mathcal{M}}\, \big\|(H_0+1)^{-1}\big\|_2^2\, \overline{m}\, \|\mathbb{1}\|^2_{\mathcal{B}\left(W_\Gamma^{1,2},L^4\right)} \|U - V\|_{L^2},
$$

for all $U, V \in \mathcal{M}$, where $\mathcal{M}$ is any bounded set in $L^2(\Omega)$, $\rho_\mathcal{M}$ is the number (3.22), and $\boldsymbol{L}_{1,\rho_\mathcal{M}}$ is the Lipschitz constant from Definition 2.15.

Proof. Using (5.1), one gets

$$
\begin{aligned}
\big\|\tilde{\mathcal{N}}(U) - \tilde{\mathcal{N}}(V)\big\|_{L^1} &= \sup_{\|W\|_{L^\infty}=1} \big|\langle \tilde{\mathcal{N}}(U) - \tilde{\mathcal{N}}(V), W\rangle\big| \\
&= \sup_{\|W\|_{L^\infty}=1} \Big|\mathrm{tr}\big[\big(f(H_U) - f(H_V)\big)W\big]\Big| \le \big\|f(H_U) - f(H_V)\big\|_1.
\end{aligned}
$$

Now the assertion follows from Lemma 4.1. □

5.18. Lemma. *We abbreviate $H_1 = H_0+1$. Let X satisfy the suppositions of Lemma 5.5. If for some U, V from $L^2(\Omega)$ there is $\tilde{N}(U) \in X$ and $\tilde{N}(V) \in X$, then*

$$(5.43)\quad \|\tilde{N}(U) - \tilde{N}(V)\|_X \le 4\left(1-\frac{d}{4}\right)^{-2} \boldsymbol{L}_{3,\rho_{\mathcal{M}}} \|H_1^{-1}\|_2^2 \|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)} \sup_{W\in K} \|H_1^{-1} W H_1^{-1}\| \cdot \max_{T\in\mathcal{M}} \|(H_T-\rho)^{-1}H_1\|^3 \|U-V\|_{L^2},$$

where $\mathcal{M} = \{U,V\}$, $\rho_{\mathcal{M}}$ is the number (3.22), and $\boldsymbol{L}_{1,\rho_{\mathcal{M}}}$ is the Lipschitz constant from Definition 2.15. Moreover,

$$(5.44)\quad \|\tilde{N}(U) - \tilde{N}(V)\|_X \le 3\left(1-\frac{d}{4}\right)^{-1} \boldsymbol{L}_{2,\rho_{\mathcal{M}}} \|H_1^{-1}\|_2 \|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)} \sup_{W\in K} \|H_1^{-1} W H_1^{-1}\|_2 \cdot \max_{T\in\mathcal{M}} \|(H_T-\rho)^{-1}H_1\|^3 \|U-V\|_{L^2}.$$

Proof. We use (5.9) for the proof and write:

$$(5.45)\qquad \|\tilde{N}(U) - \tilde{N}(V)\|_X = \sup_{W\in K} \left|\operatorname{tr}\left[\big(f(H_U) - f(H_V)\big)W\right]\right|.$$

Chosing $k=2$ or $k=3$ and $\rho \le \rho_{\mathcal{M}}$ one may continue

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

Observing the Definition 2.15 of $\boldsymbol{L}_{k,\rho}$, Theorem 2.27 and (3.8) provide

$$(5.46)\qquad \|f(H_V)(H_V-\rho)^k\|_2 \le \boldsymbol{L}_{k,\rho}\|(H_V-\rho)^{-1}\|_2 \le \boldsymbol{L}_{k,\rho}\left(1-\frac{d}{4}\right)^{-1}\|H_1^{-1}\|_2,$$

while the Birman–Solomjak Theorem 2.28 and (3.26) yield

$$\begin{aligned}
(5.47)\quad \|f(H_U)(H_U-\rho)^k - f(H_V)(H_V-\rho)^k\|_2 &\le \boldsymbol{L}_{k,\rho}\|(H_U-\rho)^{-1} - (H_V-\rho)^{-1}\|_2 \\
&\le \left(1-\frac{d}{4}\right)^{-2}\boldsymbol{L}_{k,\rho}\|H_1^{-1}\|_2 \|H_1^{-\frac12}\|_{\mathcal{B}(L^{\frac43},L^2)} \|H_1^{-\frac12}\|_{\mathcal{B}(L^2,L^4)}\|U-V\|_{L^2} \\
&\le \left(1-\frac{d}{4}\right)^{-2}\boldsymbol{L}_{k,\rho}\|H_1^{-1}\|_2 \|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}\|U-V\|_{L^2}.
\end{aligned}$$

Indeed, it is easy to see that

$$\|H_1^{-\frac12}\|_{\mathcal{B}(L^{\frac43},L^2)} \|H_1^{-\frac12}\|_{\mathcal{B}(L^2,L^4)} = \|H_1^{-1}\|_{\mathcal{B}(L^{\frac43},L^4)}, \le \|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)},$$

where the estimate follows from the Riesz–Thorin theorem via interpolation with $\frac12$ between $H_1^{-1} : L^1 \mapsto L^2$ and its adjoint $H_1^{-1} : L^2 \mapsto L^\infty$.

For the proof of (5.43) we specify $k = 3$ and observe that

$$(5.48)\quad \begin{aligned}&(H_U-\rho)^{-2}W(H_U-\rho)^{-1}-(H_V-\rho)^{-2}W(H_V-\rho)^{-1}\\ &\quad=(H_U-\rho)^{-2}W\big((H_U-\rho)^{-1}-(H_V-\rho)^{-1}\big)\\ &\qquad+(H_U-\rho)^{-1}\big((H_U-\rho)^{-1}-(H_V-\rho)^{-1}\big)W(H_V-\rho)^{-1}\\ &\qquad\quad+\big((H_U-\rho)^{-1}-(H_V-\rho)^{-1}\big)(H_V-\rho)^{-1}W(H_V-\rho)^{-1}.\end{aligned}$$

Rewriting $(H_U-\rho)^{-1}-(H_V-\rho)^{-1}$ as $(H_U-\rho)^{-1}(V-U)(H_V-\rho)^{-1}$ and using (3.8), one may estimate the Hilbert Schmidt norm of (5.48)

$$(5.49)\quad \begin{aligned}&\big\|(H_U-\rho)^{-2}W(H_U-\rho)^{-1}-(H_V-\rho)^{-2}W(H_V-\rho)^{-1}\big\|_2 \le 3\big(1-\frac{d}{4}\big)^{-1}\\ &\quad\cdot\max_{T\in\mathcal{M}}\|(H_T-\rho)^{-1}H_1\|^3\,\|H_1^{-1}\|_2\|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}\|H_1^{-1}WH_1^{-1}\|\,\|U-V\|_{L^2}.\end{aligned}$$

N.B. $\|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}=\|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)}$. Finally we estimate

$$(5.50)\qquad \big\|(H_U-\rho)^{-2}W(H_U-\rho)^{-1}\big\|_2\le\|(H_U-\rho)^{-1}H_1\|^3\|H_1^{-1}\|_2\|H_1^{-1}WH_1^{-1}\|$$

and fit together (5.45), (5.46), (5.47), (5.49), and (5.50) to get the assertion (5.43).

In order to show (5.44), we proceed in a similar way as above. One again starts with (5.45) this time specifying $k = 2$. We assemble (5.46) and the following estimates

$$\begin{aligned}&\big\|f(H_U)(H_U-\rho)^2-f(H_V)(H_V-\rho)^2\big\|_2\le\boldsymbol{L}_{2,\rho}\big\|(H_U-\rho)^{-1}(V-U)\,(H_V-\rho)^{-1}\big\|_2\\ &\quad\le\big(1-\frac{d}{4}\big)^{-1}\boldsymbol{L}_{2,\rho}\,\|H_1^{-1}\|_2\,\|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}\,\|H_1(H_V-\rho)\|\,\|U-V\|_{L^2},\end{aligned}$$

$$\begin{aligned}&\big\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1}-(H_V-\rho)^{-1}W(H_V-\rho)^{-1}\big\|_2\\ &\quad\le 2\max_{T\in\mathcal{M}}\big\|(H_T-\rho)^{-1}H_1\big\|^3\,\|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}\,\|H_1^{-1}WH_1^{-1}\|_2\,\|U-V\|_{L^2},\end{aligned}$$

$$\big\|(H_U-\rho)^{-1}W(H_U-\rho)^{-1}\big\|_2\le\|(H_U-\rho)^{-1}H_1\|^2\,\|H_1^{-1}WH_1^{-1}\|_2$$

to conclude (5.44). □

5.19. Remark. In dependence from the space dimension d and the target space X one has to ensure that

$$\sup_{W\in K}\|(H_0+1)^{-1}W(H_0+1)^{-1}\|\qquad\text{or}\qquad\sup_{W\in K}\|(H_0+1)^{-1}W(H_0+1)^{-1}\|_2$$

is finite. We will have to do this in the sequel.

5.20. Proposition. *The mapping $V\longmapsto\tilde{\mathcal{N}}(V)$ is boundedly Lipschitz continuous from $L^2(\Omega)$ into $X=C(\overline{\Omega})$. If $p\ge 2$ is chosen, such that the operator H_0+1 provides an isomorphism between the spaces $W^{1,p}_\Gamma(\Omega)$ and $W^{-1,p}_\Gamma(\Omega)$, then the mapping $\tilde{\mathcal{N}}:L^2(\Omega)\longmapsto X=W^{1,p}_\Gamma(\Omega)$ is also Lipschitz continuous on bounded subsets of $L^2(\Omega)$.*

Let $\mathcal{M}\subset L^2(\Omega)$ be bounded and $\rho\le\rho_{\mathcal{M}}$ as in (3.22); we abbreviate again $H_1=H_0+1$. The local Lipschitz constants, corresponding to $\mathcal{M}$, are in the case $d=3$

$$(5.51)\qquad 64\,\boldsymbol{L}_{3,\rho}\,\|H_1^{-1}\|_2^2\,\|H_1^{-1}\|^3_{\mathcal{B}(L^1,L^2)}\sup_{V\in\mathcal{M}}\big\|(H_V-\rho)^{-1}H_1\big\|^3$$

for $X=C(\overline{\Omega})$ and

$$(5.52)\qquad 128\,\boldsymbol{L}_{3,\rho}\,\|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}_\Gamma)}\,\|H_1^{-1}\|_2^2\,\|H_1^{-1}\|^2_{\mathcal{B}(L^1,L^2)}\sup_{V\in\mathcal{M}}\big\|(H_V-\rho)^{-1}H_1\big\|^3$$

for $X = W^{1,p}_\Gamma(\Omega)$. *In the case* $d = 1$ *or* $d = 2$, *the local Lipschitz constants are*

$$(5.53)\quad 3\left(1-\frac{d}{4}\right)^{-1}\boldsymbol{L}_{2,\rho}\,\|H_1^{-1}\|_2\,\|H_1^{-\frac{2}{3}}\|_2\,\|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}\,\|H_1^{-\frac{2}{3}}\|^2_{\mathcal{B}(L^2,L^\infty)} \cdot \sup_{V\in\mathcal{M}}\left\|(H_V-\rho)^{-1}H_1\right\|^3 \qquad for \quad X = C(\overline{\Omega})$$

$$(5.54)\quad 6\left(1-\frac{d}{4}\right)^{-1}\boldsymbol{L}_{2,\rho}\,\|H_1^{-1}\|_2\,\|H_1^{-\frac{2}{3}}\|_2\,\|H_1^{-1}\|_{\mathcal{B}(L^1,L^2)}\,\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,W^{1,q}_\Gamma)}\,\|H_1^{-\frac{2}{3}}\|_{\mathcal{B}(L^2,L^\infty)} \cdot \sup_{V\in\mathcal{M}}\left\|(H_V-\rho)^{-1}H_1\right\|^3 \qquad for \quad X = W^{1,q}_\Gamma \quad with \quad q\in\left[2,\frac{3p}{p+1}\right].$$

Proof. We use (5.43) or (5.44) from Lemma 5.18. For $X = W^{1,q}_\Gamma$ this is possible, because L^∞ is dense in $W^{-1,q'}_\Gamma$, $\left(\frac{1}{q}+\frac{1}{q'}=1\right)$, hence, $X = W^{1,q}_\Gamma$ satisfies the assumptions of Lemma 5.5. Concerning $X = C(\overline{\Omega})$, we know already from Proposition 5.8 that $\tilde{\mathcal{N}}(U)$, $\tilde{\mathcal{N}}(V)$ do belong to this space, if U, V are from $L^2(\Omega)$. Moreover, for elements $h \in C(\overline{\Omega})$ there is

$$\|h\|_{C(\overline{\Omega})} = \sup\left\{\left|\int_\Omega W(x)\,h(x)\,dx\right| \;:\; W\in L^\infty, \|W\|_{X^*} = \int |W|dx = 1\right\}.$$

Thus Remark 5.6 applies and we can use Lemma 5.18.

First we will treat the case $d = 3$ and estimate the terms

$$\sup_{W\in L^1\cap L^\infty,\|W\|_{L^1}=1}\|H_1^{-1}WH_1^{-1}\| \qquad\text{and}\qquad \sup_{W\in W^{-1,p'}_\Gamma\cap L^\infty,\ \|W\|_{W^{-1,p'}_\Gamma}=1}\|H_1^{-1}WH_1^{-1}\|,$$

where $\frac{1}{p}+\frac{1}{p'}=1$. On the one hand, one has

$$(5.55)\qquad \sup_{W\in L^1\cap L^\infty,\|L^1\|=1}\|H_1^{-1}WH_1^{-1}\| \le \|H_1^{-1}\|^2_{\mathcal{B}(L^2,L^\infty)}.$$

On the other hand, for every $W \in W^{-1,p'}_\Gamma \cap L^\infty$ with $\|W\|_{W^{-1,p'}_\Gamma} = 1$ there is

$$\|H_1^{-1}WH_1^{-1}\| = \sup_{\|\psi\|_{L^2}=\|\tilde{\psi}\|_{L^2}=1}\left|\langle H_1^{-1}WH_1^{-1}\psi,\tilde{\psi}\rangle\right|$$

and

$$\begin{aligned}\left|\langle H_1^{-1}WH_1^{-1}\psi,\tilde{\psi}\rangle\right| &= \left|\langle WH_1^{-1}\psi, H_1^{-1}\tilde{\psi}\rangle\right| = \left|\int_\Omega W(x)\big(H_1^{-1}\psi\big)(x)\big(H_1^{-1}\tilde{\psi}\big)^*(x)\,dx\right|\\ &\le \left\|\big(H_1^{-1}\psi\big)\big(H_1^{-1}\tilde{\psi}\big)^*\right\|_{W^{1,p}_\Gamma} \le \|H_1^{-1}\psi\|_{L^\infty}\|H_1^{-1}\tilde{\psi}\|_{W^{1,p}_\Gamma} + \|H_1^{-1}\tilde{\psi}\|_{L^\infty}\|H_1^{-1}\psi\|_{W^{1,p}_\Gamma}\\ &\le 2\,\|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)}\|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}_\Gamma)}.\end{aligned}$$

Hence,

$$(5.56)\qquad \sup_{W\in W^{-1,p'}_\Gamma\cap L^\infty,\ \|W\|_{W^{-1,p'}_\Gamma}=1}\|H_1^{-1}WH_1^{-1}\| \le 2\,\|H_1^{-1}\|_{\mathcal{B}(L^2,L^\infty)}\|H_1^{-1}\|_{\mathcal{B}(L^2,W^{1,p}_\Gamma)}.$$

Now combining the inequalities (5.43) and (5.55), one obtains (5.51). Analoguously, (5.43) and (5.56) yield (5.52).

In the case $d = 1$ or $d = 2$, (5.53) and (5.54) immediately follow from (5.44) in Lemma 5.18 with the inequality

$$\|H_1^{-1} W H_1^{-1}\|_2 \le \|H_1^{-\frac{1}{3}}\|_4^2 \|H_1^{-\frac{2}{3}} W H_1^{-\frac{2}{3}}\|$$

and (5.17), (5.18) from Lemma 5.7. □

5.21. Remark. In fact, it can be proved that $\tilde{\mathcal{N}} : L^2 \mapsto W_\Gamma^{1,q}$ is locally Lipschitz continuous for all $q \in [2, p]$ also in the case $d = 2$, but the occuring Lipschitz constants are worse. In our context, however, it is only essential to know, that there is at all a $q > 2$, such that $\tilde{\mathcal{N}} : L^2 \mapsto W_\Gamma^{1,q}$ is locally Lipschitz continuous and to have a fairly good constant at hand. That is why we have focused our attention to the case considered in Proposition 5.20.

The proof of the next theorem follows directly from Definition 2.16, Proposition 4.2, and Proposition 5.20.

5.22. Theorem. *Let X be any of the function spaces specified in Proposition 5.20. The mappings $\mathcal{N}_\varsigma : L^2(\Omega) \mapsto X$, $\varsigma \in \{1, \dots, \sigma\}$, are locally Lipschitz continuous. If $\mathcal{M}$ is a bounded set from $L^2(\Omega)$, then the local Lipschitz constant of $\mathcal{N}_\varsigma$ on $\mathcal{M}$ is*

$$\mathbf{Lip}_{\mathcal{M}}(\mathcal{N}_\varsigma) \le \left(1 + |\Omega|^{\frac{1}{2}} \mathbf{Lip}_{\mathcal{M}}(\mathcal{E}_{F,\varsigma})\right) \mathbf{Lip}_{\left(\mathcal{M}+\mathcal{E}_F(\mathcal{M})\chi_\Omega\right)}(\tilde{\mathcal{N}}_\varsigma),$$

where $\mathbf{Lip}_{\mathcal{M}}(\mathcal{E}_{F,\varsigma})$ is the local Lipschitz constant of the Fermi level $\mathcal{E}_{F,\varsigma}$ on the set $\mathcal{M}$ which has been estimated in the proof of of Proposition 4.2, and $\mathbf{Lip}_{\left(\mathcal{M}+\mathcal{E}_F(\mathcal{M})\chi_\Omega\right)}(\tilde{\mathcal{N}}_\varsigma)$ is the local Lipschitz constant of $\tilde{\mathcal{N}}_\varsigma : L^2(\Omega) \mapsto X$ on the bounded set $\mathcal{M} + \mathcal{E}_F(\mathcal{M})\chi_\Omega \subset L^2(\Omega)$, which has been estimated in Proposition 5.20.

5.e. **Monotonicity.**

5.23. Theorem. *We refer to the notation of Definition 2.16. For any $\varsigma \in \{1, \dots, \sigma\}$ the negative particle density operator $-\mathcal{N}_\varsigma$ is a monotone operator from $L^2(\Omega)$ into $L^2(\Omega)$ and a strictly monotone operator from $W_\Gamma^{1,2}(\Omega)$ into $W_\Gamma^{-1,2}(\Omega)$.*

The proof of these monotonicity properties is similar to that given in [12, 35, 36]. It is based on the Fréchet differentiability of the particle density operator $\mathcal{N}_\varsigma$ and explicit calculation of

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

The resulting expression turns out positive due to the monotonicity properties of the distribution function f_ς, cf. Assumption 2.14.

6. Existence of solutions and apriori estimates

6.a. **The linear Poisson operator.**

6.1. Lemma. *The operator $A : W_{\hat{\Gamma}}^{1,2}(\hat{\Omega}) \mapsto W_{\hat{\Gamma}}^{-1,2}(\hat{\Omega})$ from Definition 2.22 is strongly monotone and Lipschitz continuous.*

$$m_A = c_b^{-1} \min\left\{1, \operatorname*{vraimin}_{x\in\hat{\Omega}} \operatorname{spec}[\varepsilon(x)]\right\} \tag{6.1}$$

serves as a monotonicity constant and

$$M_A = \operatorname*{vraimax}_{x\in\hat{\Omega}} \operatorname{spec}[\varepsilon(x)] + \|b\|_{L^\infty(\partial\hat{\Omega}\setminus\hat{\Gamma})} \|\mathbb{1}\|^2_{\mathcal{B}(W_{\hat{\Gamma}}^{1,2}(\hat{\Omega}), L^2(\partial\hat{\Omega}\setminus\hat{\Gamma}))}, \tag{6.2}$$

as a Lipschitz constant, where $\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\hat\Gamma}(\hat\Omega),L^2(\partial\hat\Omega\setminus\hat\Gamma))}$ *denotes the embedding constant from* $W^{1,2}_{\hat\Gamma}(\hat\Omega)$ *into* $L^2(\partial\hat\Omega\setminus\hat\Gamma)$.

Proof. First we observe

$$\begin{aligned}\|\operatorname{grad} u\|^2_{L^2(\hat\Omega,\mathbb{R}^d)} &= \|\varepsilon^{-\frac12}\varepsilon^{\frac12}\operatorname{grad} u\|^2_{L^2(\hat\Omega,\mathbb{R}^d)} \le \|\varepsilon^{-1}\|_{L^\infty(\hat\Omega,\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}\|\varepsilon^{\frac12}\operatorname{grad} u\|^2_{L^2(\hat\Omega,\mathbb{R}^d)}\\ &= \|\varepsilon^{-1}\|_{L^\infty(\hat\Omega,\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}\int_{\hat\Omega}\langle\varepsilon(x)\operatorname{grad} u(x),\operatorname{grad} u(x)\rangle\,dx.\end{aligned}$$

Now one easily deduces from the definition of A and c_b (cf. Definition 2.22)

$$\begin{aligned}\|u\|^2_{W^{1,2}_{\hat\Gamma}(\hat\Omega)} &\le c_b\big(\|\operatorname{grad} u\|^2_{L^2(\hat\Omega,R^d)} + \|bu^2\|_{L^1(\partial\hat\Omega\setminus\hat\Gamma)}\big)\\ &\le c_b\Big(\|\varepsilon^{-1}\|_{L^\infty(\hat\Omega,\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}\int_{\hat\Omega}\langle\varepsilon(x)\operatorname{grad} u(x),\operatorname{grad} u(x)\rangle\,dx + \int_{\partial\hat\Omega\setminus\hat\Gamma} b(\tau)u^2(\tau)\,d\tau\Big)\\ &\le c_b\max\big\{1,\|\varepsilon^{-1}\|_{L^\infty(\hat\Omega,\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}\big\}\,\langle Au,u\rangle.\end{aligned}$$

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

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

by means of

$$\begin{aligned}\big|\langle Au,v\rangle\big| &= \Big|\int_{\hat\Omega}\langle\varepsilon^{\frac12}(x)\operatorname{grad} u(x),\varepsilon^{\frac12}(x)\operatorname{grad} v(x)\rangle dx + \int_{\partial\hat\Omega\setminus\hat\Gamma} b(\tau)\,u(\tau)\,v(\tau)\,d\tau\Big|\\ &\le \|\varepsilon\|_{L^\infty(\hat\Omega,\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}\|u\|_{W^{1,2}_{\hat\Gamma}(\hat\Omega)}\|v\|_{W^{1,2}_{\hat\Gamma}(\hat\Omega)} + \|b\|_{L^\infty(\partial\hat\Omega\setminus\hat\Gamma)}\|u\|_{L^2(\partial\hat\Omega\setminus\hat\Gamma)}\|v\|_{L^2(\partial\hat\Omega\setminus\hat\Gamma)}.\end{aligned}$$

Finally one observes that $W^{1,2}_{\hat\Gamma}(\hat\Omega)$ embeds continuously into $L^2(\partial\hat\Omega\setminus\hat\Gamma)$. □

6.b. **The nonlinear Schrödinger–Poisson operator.** Up to now we have regarded the particle density operators as operators from $L^2(\Omega)$ into function spaces over Ω. 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 $\hat\Omega$ by means of the identification operators Z^*_ς from Definition 2.23. In the following $\mathbf{V} = (V_1,\dots,V_\sigma) \in L^2(\Omega,\mathbb{R}^\sigma)$ is a given σ–tuple of external potentials.

The statements of the next proposition follow directly from Theorem 5.23 and the Lipschitz properties of the operators $\mathcal{N}_\varsigma$ (cf. §5.d).

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

$$L^2(\hat\Omega)\ni V\longmapsto -Z^*_\varsigma\mathcal{N}_\varsigma(V_\varsigma+Z_\varsigma V)\in L^2(\hat\Omega)$$

is monotone from $L^2(\hat\Omega)$ *into itself and also monotone from* $W^{1,2}_{\hat\Gamma}(\hat\Omega)$ *into* $W^{-1,2}_{\hat\Gamma}(\hat\Omega)$. *Moreover, this operator is locally Lipschitz continuous from* $L^2(\hat\Omega)$ *into* $L^2(\hat\Omega)$, *and its local Lipschitz constant on a bounded set* $\widehat{\mathcal{M}}\subset L^2(\hat\Omega)$ *is*

$$\|Z^*_\varsigma\|^2_{\mathcal{B}(L^2(\Omega),L^2(\hat\Omega))}\mathbf{Lip}_{(V_\varsigma+Z_\varsigma\widehat{\mathcal{M}})}(\mathcal{N}_\varsigma), \tag{6.3}$$

where $\mathbf{Lip}_{(V_\varsigma+Z_\varsigma\widehat{\mathcal{M}})}(\mathcal{N}_\varsigma)$ *is the local Lipschitz constant of the mapping* $\mathcal{N}_\varsigma : L^2(\Omega)\mapsto L^2(\Omega)$, *restricted to the set* $V_\varsigma+Z_\varsigma\widehat{\mathcal{M}}$.

Proposition 6.2 implies by means of Theorem 2.26 the following

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

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

is strongly monotone with m_A as a monotonicity constant. Additionally, this operator is locally Lipschitz continuous. More precisely: if $\widehat{\mathcal{M}}_1$ is a bounded set in $W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})$ and $\widehat{\mathcal{M}}$ denotes the image of $\widehat{\mathcal{M}}_1$ under the canonical embedding from $W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})$ into $L^2(\hat{\Omega})$, then the local Lipschitz constant of $P_{\mathbf{V}}$, corresponding to the set $\widehat{\mathcal{M}}_1$, may be taken as

$$\begin{aligned}\mathbf{Lip}_{\widehat{\mathcal{M}}_1}(P_{\mathbf{V}}) = M_A &+ \sum_{\varsigma \in \{1,\dots,\sigma\}} \mathbf{Lip}_{\widehat{\mathcal{M}}_1}(F_\varsigma) \\ &+ \|\mathbb{1}\|^2_{\mathcal{B}(W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}),L^2(\hat{\Omega}))} \sum_{\varsigma \in \{1,\dots,\sigma\}} \|Z^*_\varsigma\|^2_{\mathcal{B}(L^2(\Omega),L^2(\hat{\Omega}))} \mathbf{Lip}_{(V_\varsigma + Z_\varsigma \widehat{\mathcal{M}})}(\mathcal{N}_\varsigma).\end{aligned} \tag{6.5}$$

$\mathbf{Lip}_{\widehat{\mathcal{M}}_1}(F_\varsigma)$ is the local Lipschitz constant of the mapping F_ς defined in Assumption 2.10. The nonlinear Poisson equation

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

admits exactly one solution $\underline{V}$ for every effective doping profile $D \in W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})$ (cf. Definition 2.23). This solution satisfies the estimate

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

If $\mathcal{J} : W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}) \mapsto W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})$ is the duality mapping and M_P the local Lipschitz constant (6.5) *of the mapping $P_{\mathbf{V}}$ which corresponds to the centered ball $\widehat{\mathcal{M}}_1$ in $W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})$ with radius*

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

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

$$Q_{\mathbf{V}} : \widehat{\mathcal{M}}_1 \longmapsto \widehat{\mathcal{M}}_1, \qquad Q_{\mathbf{V}} : V \longmapsto V - \frac{m_A}{M_P^2} \mathcal{J}^{-1}(P_{\mathbf{V}} V - D), \tag{6.9}$$

which is contractive on $\widehat{\mathcal{M}}_1$ with the contraction constant

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

From Proposition 6.3 one easily deduces

6.4. Theorem. *The Schrödinger–Poisson system without exchange–correlation potential (cf. Definition 2.23) has the unique solution $(\underline{V}, \tilde{\mathcal{N}}_1(V_1 + \underline{V}), \dots, \tilde{\mathcal{N}}_\sigma(V_\sigma + \underline{V}))$, where $\underline{V}$ is the fixed point of the operator* (6.9).

6.5. Remark. It is not hard 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, then satisfies similar monotonicity and Lipschitz properties and the machinery on monotone operators still works.

Next we will have a look on the dependance of the solution of the nonlinear Schrödinger–Poisson equation (6.6) on the vector $\mathbf{V} = (V_1, \dots, V_\sigma) \in L^2(\Omega, \mathbb{R}^\sigma)$ of external potentials.

6.6. Lemma. *Let*

$$\mathcal{L} : L^2(\Omega, \mathbb{R}^\sigma) \longmapsto L^2(\hat{\Omega}), \qquad \mathcal{L}(\mathbf{V}) = \underline{V} \tag{6.11}$$

be the operator, which assigns to the σ–tuple of external potentials $\mathbf{V} = (V_1, \dots, V_\sigma) \in L^2(\Omega, \mathbb{R}^\sigma)$ the solution $\underline{V}$ of the equation (6.6). If $\mathcal{M}$ is a bounded set in $L^2(\Omega)$, then

$$\sup_{\mathbf{V} \in \mathcal{M}^\sigma} \|\mathcal{L}(\mathbf{V})\|_{L^2(\hat{\Omega})} \leq \frac{\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}), L^2(\hat{\Omega}))}}{m_A} \Bigg(q \, \|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}), L^2(\hat{\Omega}))} \|N_A - N_D\|_{L^2(\hat{\Omega})} + \|\varepsilon\|_{L^\infty(\hat{\Omega}, \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d))} \|\varphi_{\hat{\Gamma}}\|_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})} + \sum_{\varsigma \in \{1, \dots, \sigma\}} \|F_\varsigma(0)\|_{W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})} + \sup_{\mathbf{V} = (V_1, \dots, V_\sigma) \in \mathcal{M}^\sigma} \sum_{\varsigma \in \{1, \dots, \sigma\}} \left\| Z_\varsigma^* \mathcal{N}_\varsigma(V_\varsigma) \right\|_{W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})} \Bigg). \tag{6.12}$$

The mapping $\mathcal{L}$ is boundedly Lipschitz continuous from $L^2(\Omega, \mathbb{R}^\sigma)$ into $W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})$, and its local Lipschitz constant corresponding to $\mathcal{M}^\sigma$ is

$$\frac{2}{m_A} \|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\hat{\Gamma}}(\hat{\Omega}), L^2(\hat{\Omega}))} \sup_{\varsigma \in \{1, \dots, \sigma\}} \|Z_\varsigma^*\|_{\mathcal{B}(L^2(\Omega), L^2(\hat{\Omega}))} \sum_{\varsigma \in \{1, \dots, \sigma\}} \mathbf{Lip}_{(\mathcal{M} + Z_\varsigma \mathcal{L}(\mathcal{M}^\sigma))}(\mathcal{N}_\varsigma), \tag{6.13}$$

where $\mathbf{Lip}_{(\mathcal{M} + Z_\varsigma \mathcal{L}(\mathcal{M}^\sigma))}(\mathcal{N}_\varsigma)$ is the local Lipschitz constant of the mapping $\mathcal{N}_\varsigma : L^2(\Omega) \mapsto L^2(\Omega)$, 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 (2.16), and the inequality

$$\|\tilde{\varphi}_{\hat{\Gamma}}\|_{W^{-1,2}_{\hat{\Gamma}}(\hat{\Omega})} \leq \|\varepsilon\|_{L^\infty(\hat{\Omega}, \mathcal{B}(\mathbb{R}^d, \mathbb{R}^d))} \|\varphi_{\hat{\Gamma}}\|_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})}$$

this implies the first assertion.

For the proof of the local Lipschitz continuity, let $\mathbf{U} = (U_1, ..., U_\sigma)$ and $\mathbf{V} = (V_1, ..., V_\sigma)$ 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,

$$\begin{aligned} \|\mathcal{L}(\mathbf{U}) - \mathcal{L}(\mathbf{V})\|_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})} &= \|Q_\mathbf{U}\mathcal{L}(\mathbf{U}) - Q_\mathbf{V}\mathcal{L}(\mathbf{V})\|_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})} \\ &\leq \|Q_\mathbf{U}\mathcal{L}(\mathbf{U}) - Q_\mathbf{U}\mathcal{L}(\mathbf{V})\|_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})} + \|(Q_\mathbf{U} - Q_\mathbf{V})\mathcal{L}(\mathbf{V})\|_{W^{1,2}_{\hat{\Gamma}}(\hat{\Omega})} \end{aligned}$$

Taking into account the Lipschitz constant for $Q_\mathbf{U}$, given in (6.10), one easily deduces from this

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

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

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

one arrives at

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

and finally at the Lipschitz constant (6.13). □

6.c. **The Kohn–Sham system.** We will now introduce an adequate subset of $L^1(\Omega,\mathbb{R}^\sigma)$ 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.

6.7. Definition. Let $\mathbf{V}=(V_1,\dots,V_\sigma)\in L^2(\Omega,\mathbb{R}^\sigma)$ be a given σ–tuple of external potentials and $N_1,\dots,N_\sigma$, the fixed numbers of carriers, cf. Definition 2.16. We define

$$L^1_N=\Big\{\mathbf{u}=(u_1,\dots,u_\sigma): u_\varsigma\ge 0,\ \int u_\varsigma(x)dx=N_\varsigma,\ \varsigma\in\{1,\dots,\sigma\}\Big\} \tag{6.14}$$

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

$$\Phi_\varsigma(\mathbf{u})=\mathcal{N}_\varsigma\Big(V_\varsigma+V_{xc,\varsigma}(\mathbf{u})+Z_\varsigma\mathcal{L}\big(V_1+V_{xc,1}(\mathbf{u}),\dots,V_\sigma+V_{xc,\sigma}(\mathbf{u})\big)\Big). \tag{6.15}$$

6.8. Lemma. *For any $\varsigma\in\{1,\dots,\sigma\}$ let $V_{xc,\varsigma}$ be a bounded and continuous mapping from $\big(L^1(\Omega)\big)^\sigma$ into $L^2(\Omega)$. If*

$$\delta=\sup_{\varsigma\in\{1,\dots,\sigma\}}\sup_{\mathbf{u}\in L^1_N}\big\|V_{xc,\varsigma}(\mathbf{u})\big\|_{L^2(\Omega)} \tag{6.16}$$

and

$$\mathcal{M}=\Big\{V\in L^2(\Omega):\max_{\varsigma\in\{1,\dots,\sigma\}}\|V-V_\varsigma\|_{L^2(\Omega)}\le\delta\Big\}, \tag{6.17}$$

then the number

$$\begin{aligned}
s=\sup_{\varsigma\in\{1,\dots,\sigma\}}\|V_\varsigma\|_{L^2(\Omega)}+\delta+\Big(\sup_{\varsigma\in\{1,\dots,\sigma\}}\|Z_\varsigma\|_{\mathcal{B}(L^2(\hat\Omega),L^2(\Omega))}\Big)\frac{\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\hat\Gamma}(\hat\Omega),L^2(\hat\Omega))}}{m_A}\\
\cdot\Bigg(q\,\|\mathbb{1}\|_{\mathcal{B}(W^{1,2}_{\hat\Gamma}(\hat\Omega),L^2(\hat\Omega))}\|N_A-N_D\|_{L^2(\hat\Omega)}+\|\varepsilon\|_{L^\infty(\hat\Omega,\mathcal{B}(\mathbb{R}^d,\mathbb{R}^d))}\|\varphi_{\hat\Gamma}\|_{W^{1,2}_{\hat\Gamma}(\hat\Omega)}\\
+\sum_{\varsigma\in\{1,\dots,\sigma\}}\|F_\varsigma(0)\|_{W^{-1,2}_{\hat\Gamma}(\hat\Omega)}+\sum_{\varsigma\in\{1,\dots,\sigma\}}\sup_{V\in\mathcal{M}}\big\|Z_\varsigma^*\mathcal{N}_\varsigma(V)\big\|_{W^{-1,2}_{\hat\Gamma}(\hat\Omega)}\Bigg)
\end{aligned} \tag{6.18}$$

is a common upper bound for the $L^2(\Omega)$–norm of the Schrödinger potentials which are involved in the definition of the carrier densities in (6.15)*, and*

$$\rho = -\left(1 - \frac{d}{4}\right)\gamma_2^{\frac{8}{4-d}} \sup_{\varsigma\in\{1,\dots,\sigma\}} \overline{m}_\varsigma^{\frac{d}{4-d}} s^{\frac{4}{4-d}} - 1 \tag{6.19}$$

is the corresponding quantity (3.22)*. Any element from the range of Φ does not only belong to L^1_N, but satisfies the a priori estimates given in Proposition 5.8, Corollary 5.9, and Proposition 5.10, where the s–ball in $L^2(\Omega)$ serves as the set $\mathcal{M}$ in §5.b.*

Proof. For the proof it suffices to show that s is an $L^2(\Omega)$–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 to apply Proposition 5.8, Corollary 5.9, and Proposition 5.10 respectively. (6.16) implies

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

The right hand side of (6.12) provides a $L^2(\hat{\Omega})$–bound for all

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

if in (6.12) V_ς is replaced by $V_\varsigma + V_{xc,\varsigma}(\mathbf{u})$ and $\mathcal{M}$ is defined by (6.17). □

6.9. Remark. Often the exchange–correlation terms $V_{xc,\varsigma}$ are given by rational expressions as e.g. (1.10) which allow to estimate the quantity δ in Lemma 6.8 in terms of the data of the problem. If $\alpha \le \frac{1}{2}$ in (1.10) then

$$\delta \le \sup_{\varsigma\in\{1,\dots,\sigma\}} \beta_\varsigma N_\varsigma^\alpha |\Omega|^{\frac{1}{2}-\alpha}. \tag{6.20}$$

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

6.10. Theorem. *If $V_{xc,\varsigma}$ is for any $\varsigma \in \{1,\dots,\sigma\}$ a bounded and continuous mapping from $\left(L^1(\Omega)\right)^\sigma$ into $L^2(\Omega)$, then the mapping Φ from Definition 6.7 has a fixed point.*

Proof. It is evident that Φ maps L^1_N into itself (cf. Definition 6.7 and Definition 2.16). From the continuity properties of the mappings $V_{xc,\varsigma}$, $\mathcal{N}_\varsigma$, and $\mathcal{L}$ (cf. §5.d and Lemma 6.6) directly follows that Φ is continuous. Lemma 6.8 assures that the image of Φ is bounded in a space $C^\alpha(\Omega, \mathbb{R}^\sigma)$. Consequently, by the Arzela–Ascoli theorem, Φ satisfies the suppositions of Schauder's fixed point theorem, hence, it has a fixed point in L^1_N. □

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

6.12. Corollary. *The particle densities u_ς of a fixed point $\mathbf{u} = \big(u_1, \dots, u_\sigma\big)$ of Φ do not only belong to $L^1(\Omega)$, but satisfy the estimates given in Proposition 5.8, Corollary 5.9, and Proposition 5.10, where ρ is given by* (6.19).

Proof. Obviously any fixed point is contained in the image of Φ and, hence, obeys the a priori estimates stated in Lemma 6.8. □

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

$$(V, u_1, \dots, u_\sigma) = \left(A^{-1}\Big(D + \sum_{\varsigma\in\{1,\dots,\sigma\}} Z_\varsigma^* u_\varsigma\Big), u_1, \dots, u_\sigma\right) \tag{6.21}$$

is a solution of the Kohn-Sham system, cf. Definition 2.23. In particular, this means that the Kohn-Sham system always admits a solution.

Proof. It follows from Definition 6.7 and Definition 2.23 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 (6.21) a solution of the Kohn–Sham system in the sense of Definition 2.23. This follows directly from the definition of $\mathcal{L}$ in (6.11) and Corollary 6.12. □

6.14. Remark. Obviously the (homogenized) electrostatic potential

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

belongs to the intersection of a space $C^\alpha(\hat{\Omega})$ and a space $W^{1,p}_{\hat{\Gamma}}(\hat{\Omega})$ with $p > 2$. Reiterating this argument, one obtains in smooth situations — where the domain $\hat{\Omega}$ and the coefficients are smooth and the boundary conditions are not mixed — that the particle densities and the Hartree potential, of a solution are infinitly smooth.

6.15. Remark. Corollary 6.12 justifies to demand in Definition 2.23 that a solution of the Schrödinger–Poisson system has carrier densities u_ς from the space $L^2(\Omega)$.

6.16. Remark. The authors have been trying hard to find a bounded subset of a stronger topologized space than L^1 — e.g. L^2 or L^∞ — which Φ maps continuously and compactly into itself. The aim was to get a solution, which belongs a priori to a space of more regular functions. All our attempts have failed. May be it is impossible to find such a set, because there is no physically motivated growth restriction for stronger norms than the L^1–norm [23]. N.B. the L^1–norm of each carrier density is fixed by the conservation law (2.10) in Definition 2.16. The L^1–calculus for the carrier densities requires a theory of Schrödinger operators with potentials from L^2 as it has been developed in §3.

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 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 (1.10) are not Lipschitz continuous. However, the expressions (1.10) are not properly justified for very low carrier densities u_ς and the following regularization is possible [48]

$$V_{xc,\varsigma}(\mathbf{u}) = \beta_\varsigma\,\delta_\varsigma^\alpha - \beta_\varsigma\left(u_\varsigma + \delta_\varsigma\right)^\alpha, \quad \beta_\varsigma > 0, \quad 0 \le \alpha \le \frac{1}{2}. \tag{7.1}$$

This mapping $V_{xc,\varsigma} : \left(L^1(\Omega)\right)^\sigma \longmapsto L^2(\Omega)$ is Lipschitz continuous.

7.2. Theorem. *If the mappings $V_{xc,\varsigma}$ are boundedly Lipschitz continuous from $\left(L^1(\Omega)\right)^\sigma$ into $L^2(\Omega)$ on the set L^1_N, and the corresponding Lipschitz constants are suffiently small, then the solution of the Schrödinger–Poisson system is unique (cf. Definition 2.23 and Definition 6.7).*

Proof. One again regards the mapping $\Phi : L^1_N \longmapsto L^1_N$ from Definition 6.7. Combining the results on Φ from §6.c and the Lipschitz properties of the mappings $V_{xc,\varsigma}$, $\mathcal{L}$ (cf.

Lemma 6.6), Z_ς (cf. Definition 2.23), and $\mathcal{N}_\varsigma$ (cf. Theorem 5.22), one obtains that Φ is a Lipschitz continuous mapping from L^1_N into itself.

$$\mathbf{Lip}_{L^1_N}(\Phi_\varsigma) = \mathbf{Lip}_{L^1_N}(V_{xc,\varsigma})\,\mathbf{Lip}_{\mathcal{M}+Z_\varsigma\mathcal{L}(\mathcal{M})}(\mathcal{N}_\varsigma)\,\Big(1 + \big\|Z_\varsigma\big\|_{\mathcal{B}(L^2(\hat{\Omega}),L^2(\Omega))}\mathbf{Lip}_{\mathcal{M}^\sigma}(\mathcal{L})\Big)$$

is a Lipschitz constant of the ς–component (6.15) of Φ, where $\mathcal{M}$ is the set defined under (6.17). Thus, if the Lipschitz constants $\mathbf{Lip}_{L^1_N}(V_{xc,\varsigma})$ of the mappings $V_{xc,\varsigma}$ are sufficiently small, then Banachs's fixed point principle provides a unique solution of the Schrödinger–Poisson system. □

7.3. Remark. In the sense of Remark 6.9 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 6.6 and Theorem 5.22 respectively. Thus in principle one can get ranges of data which assure uniqueness. N.B. for this purpose the Birman–Solomjak Theorem 2.28 is essential, as it puts the cutting edge to our estimates. It is not known yet, however, wether the uniqueness assuring ranges of data, which are determined that way, are pessimistic or really interesting from a physical point of view.

A.1. **A few remarks on the physical background.** This section provides a physical perspective leading to the mathematical problem presented in the main text. In principle the phenomena in a bulk semiconductor and the semiconductor itself are the result of many particle interactions and as such they have to be described by many particle theory. Such theories can be formulated (cf. e. g. [11]) and reflect the full scope of high-frequency, high-field and high-excitation effects, for example intracollisional effects, quasi-particle interaction and so on. Fortunately it was possible to understand bulk semiconductors whitout external fields using comparatively simple means inasmuch the electronic band structure can be computed from a single particle Schrödinger equation with a pseudopotential [13]. Therefore the selection of a suitable mathematical model of a rather unspecified nanostructure should be "bottom - top" supplementing the re-interpreted single particle Schrödinger equation with some key features rather than deskilling the most of many body quantum theory.

The application of an electrostatic potential of 5 or 6 V to the contacts of a submicron MOSFET yields a slowly varying potential in comparision with the variation of Bloch functions: The Bloch functions are periodic with the crystal lattice having lattice constants of e. g. 0.543 nm (Si) while the gate length is still about $100\ldots 200$ nm. Therefore one is in a position to apply the effective mass approximation [2] which must be coupled to the poisson equation for self-consistency. To take into account many body effects the potential of the effective mass Schrödinger equation should contain an exchange-correlation term $V_{xc,\varsigma}(\mathbf{u})$ which is a functional of the single particle density u_ς following the local density approximation of density functional theory [44] thus achieving (1.9).

The exchange-correlation potential $V_{xc,\varsigma}(\mathbf{u})$ is again - though in principle fixed by many body quantum theory - open to sound approximations. The oldest approximation is the Slater approximation [5] yielding $V_{xc,\varsigma}(\mathbf{u}) = \text{const.}\ u_\varsigma^{1/n}$, $n = 3, 2$ in three or two space dimensions. It is accurate in three space dimensions if

$$r_s = \frac{r_0}{a_B^*} \ll 1 \qquad \text{where} \qquad r_0 = \left(\frac{3}{4\pi u_\varsigma}\right)^{1/3} \qquad \text{and} \qquad a_B^* = \left(\frac{\hbar^2}{m_0 e^2}\right)\frac{m_0}{m_\varsigma^*}\epsilon.$$

r_0 is the mean particle distance and a_B^* is the effective Bohr radius, scaled by the effective mass m_ς^* and the dielectric constant ϵ [2, S. 26].

Generally the exchange–correlation potentials $V_{xc,\varsigma}$, $\varsigma \in \{1, \ldots, \sigma\}$ are given by the functional derivatives

$$V_{xc,\varsigma} = \frac{\delta \mathbb{E}_{xc}}{\delta u_\varsigma}, \qquad \varsigma \in \{1, \ldots, \sigma\},$$

of the exchange–correlation energy $\mathbb{E}_{xc} = \mathbb{E}_{xc}(\mathbf{u})$, which is a functional of the carrier densities (cf. e.g. [37, 15]). Within the local–density approximation (LDA) the exchange–correlation energy $\mathbb{E}_{xc}$ is expressed by the exchange and correlation energy $\mathcal{E}_{xc}(\mathbf{u})$ per particle of a homogeneous electron gas (cf. e.g. [37, 15])

$$\mathbb{E}_{xc} = \int_\Omega \left(\sum_{\varsigma\in\{1,\ldots,\sigma\}} e_\varsigma u_\varsigma(\mathfrak{V}_\varsigma)(x)\right) \mathcal{E}_{xc}\left(\mathbf{u}(x)\right) dx$$

and the exchange–correlation potential becomes

$$V_{xc,\varsigma}^{LDA} = \frac{\partial}{\partial u_\varsigma}\left(\mathcal{E}_{xc}(\mathbf{u}) \sum_{\varsigma\in\{1,\dots,\sigma\}} e_\varsigma u_\varsigma(\mathfrak{V}_\varsigma)(x)\right).$$

A term often referred to for three-dimensional systems is the following one of Hedin and Lundqvist [44, S. 77]

$$\mathcal{E}_{xc}(u) = -0.045\ F(x)\ \text{Ry} \quad \text{with} \quad x = \frac{r_s}{21} \quad \text{and}$$
$$F(x) = (1+x^3)\ln\left(1+\frac{1}{x}\right) + \frac{x}{2} - x^2 - \frac{1}{3}.$$

It does not reproduce the density dependence in the high- and low-density limits. To achieve this one has to introduce parameter dependent formulæ thus entering the field of parameter determination [44]. "The search for an accurate $\mathbb{E}_{xc}$ has encountered tremendous difficulty and continues to be the greatest challenge in the density–functional theory." [37].

A.2. **Distribution functions.** In order to avoid the problems of valence band coupling [2] in the effective mass approximation a *model* of a two-band semiconductor is assumed as mentioned in the introduction. Let $\varsigma = 1$ for holes and $\varsigma = 2$ for electrons. The nanostructure in a n dimensional bulk material ($n = 3$) may be in the simplest case characterized by a set of band discontinuities $\Delta E_{\varsigma,j},\ 1 \le j \le n$ each band-edge offset being rescinded after a length L_j. Let d be the number of band discontinuities. Thus for $d = 0$ there is no nanostructure, for $d = 1$ there is a two dimensional electron gas in a quantum well, for $d = 2$ there is a one dimensional electron gas in a quantum wire and for $d = 3$ a fully quantized electron ensemble exists in a quantum dot. For $d > 1$ the separation of variables in the nanostructure is assumed. Furthermore the assumption for the band discontinuities $\Delta E_{\varsigma,j},\ j = 1,\dots,d$ is

$$\text{sign}(\Delta E_{1,j}) = -\text{sign}(\Delta E_{2,j})$$

to minimize unwanted couplings between e. g. envelope valency states and bulk conduction band states. The condition

$$E_V + \Delta E_{1,j} < E_C + \Delta E_{2,j} \qquad 1 \le j \le d$$

is self-evident.

One defines $\boldsymbol{x}_{(1)} := \{x_i\}_{i=1}^d,\ \boldsymbol{x}_{(2)} := \{x_i\}_{i=d+1}^n$ and $\boldsymbol{x} = (\boldsymbol{x}_{(1)}, \boldsymbol{x}_{(2)})$. In the same way one splits the propagation vectors $\boldsymbol{k} = (\boldsymbol{k}_{(1)}, \boldsymbol{k}_{(2)})$ with $\boldsymbol{k}_{(1)} := \{k_i\}_{i=1}^d,\ \boldsymbol{k}_{(2)} := \{k_i\}_{i=d+1}^n$. Let $\{x_i\}_{i=1}^n$ and $\{k_i\}_{i=1}^n$ be cartesian coordinates and $\{L_i\}_{i=1}^n$ a set of strictly positive finite real numbers where the $\{L_i\}_{i=1}^d$ characterize the nanostructure. One assumes that the n cartesian vectors $(0,\dots,0,L_i,0,\dots,0)$ with L_i at the i-th position are lattice vectors of the translation lattice of the bulk crystal. From effective mass theory [32] at a band edge at $\boldsymbol{k}_{0\varsigma}$ follows that the wave function is approximately given by

$$\Psi_Q(\boldsymbol{x}) = \chi_Q(\boldsymbol{x}) u_{\boldsymbol{k}_{0\varsigma}}(\boldsymbol{x}), \tag{A.1}$$

where $\chi_Q(\boldsymbol{x})$ denotes the envelope function, Q the set of quantum numbers and $u_{\boldsymbol{k}_{0\varsigma}}(\boldsymbol{x})$ is the lattice periodic Bloch function of the bulk material. Let the wave function Ψ_Q be normalized in $L_1 \times L_2 \times \cdots \times L_n$. $\chi_Q(\boldsymbol{x})$ has to fulfill the effective mass equation

$$\left(E_\varsigma(-i\boldsymbol{\nabla} + \boldsymbol{k}_0) + \mathfrak{V}_\varsigma(\boldsymbol{x}_{(1)}) - \mathcal{E}_Q\right)\chi_Q(\boldsymbol{x}) = 0$$

or, explicitely for $\boldsymbol{k}_0 = 0$

$$\left(E_\varsigma(0) - \frac{\hbar^2}{2} \sum_{i,j=1}^{n} w_{ij} \frac{\partial^2}{\partial x_i \partial x_j} + \mathfrak{V}_\varsigma(\boldsymbol{x}_{(1)}) - \mathcal{E}_Q \right) \chi_Q(\boldsymbol{x}) = 0.$$

Following the coordinate splitting one splits the reciprocal effective mass tensor also

$$\begin{aligned}
w_{ij} &:= \frac{1}{\hbar^2} \frac{\partial^2 E_\varsigma(0)}{\partial k_i \partial k_j}, \\
\boldsymbol{w} &= \begin{pmatrix} \boldsymbol{w}_{(1,1)} & \boldsymbol{w}_{(1,2)} \\ \boldsymbol{w}_{(2,1)} & \boldsymbol{w}_{(2,2)} \end{pmatrix} \quad \text{with} \\
\boldsymbol{w}_{(1,1)} &= \{w_{ij}\}_{i,j=1}^{d}, \\
\boldsymbol{w}_{(1,2)} &= \left\{ \{w_{ij}\}_{i=1}^{d} \right\}_{j=d+1}^{n}, \\
\boldsymbol{w}_{(2,1)} &= \left\{ \{w_{ij}\}_{i=d+1}^{n} \right\}_{j=1}^{d}, \\
\boldsymbol{w}_{(2,2)} &= \{w_{ij}\}_{i,j=d+1}^{n}.
\end{aligned}$$

Setting

(A.2) $$\chi_Q(\boldsymbol{x}) = \psi_{Q_{(1)}}(\boldsymbol{x}_{(1)}) \exp(-i\, {}^t\boldsymbol{k}_{(2)} \boldsymbol{w}_{(2,1)} \boldsymbol{w}_{(1,1)}^{-1} \boldsymbol{x}_{(1)}) \ \exp(i\, {}^t\boldsymbol{k}_{(2)} \boldsymbol{x}_{(2)})$$

one gets for $\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})$ the equation (cf. (1.8))

$$\left(-\frac{\hbar^2}{2} \boldsymbol{w}_{(1,1)} \frac{\partial^2}{\partial \boldsymbol{x}_{(1)} \partial \boldsymbol{x}_{(1)}} + \mathfrak{V}_\varsigma(\boldsymbol{x}_{(1)}) - \mathcal{E}'_Q \right) \psi_{Q_{(1)}}(\boldsymbol{x}_{(1)}) = 0$$

with

(A.3) $$\mathcal{E}'_Q = -E_\varsigma(0) + \mathcal{E}_{Q_{(1)}} - e_\varsigma \frac{\hbar^2}{2} {}^t\boldsymbol{k}_{(2)} (\boldsymbol{w}_{(2,2)} - \boldsymbol{w}_{(2,1)} \boldsymbol{w}_{(1,1)}^{-1} \boldsymbol{w}_{(1,2)}) \boldsymbol{k}_{(2)}.$$

Note that the choice of cartesian coordinates $\{x_i\}_{i=1}^n$ also implies cartesian propagation coordinates $\{k_i\}_{i=1}^n$ but the principal axes of the constant-energy ellipsoids have in general another orientation. Therefore the matrix $\boldsymbol{w}$ enters the foregoing expressions (cf. [3, III. A.]). As usual, all vectors are viewed as column vectors, ${}^t\boldsymbol{k}$ is the transposed propagation vector and ${}^t\boldsymbol{k}\boldsymbol{x}$ means the dual pairing between propagation and position vectors.

The carrier density $u_\varsigma(\boldsymbol{x}, t)$ is given by the trace of the statistical operator $\hat{W}_\varsigma$ [9, S. 85/86] with $\delta(\boldsymbol{r} - \boldsymbol{x})$:

$$u_\varsigma(\boldsymbol{x}, t) = \operatorname{tr}(\delta(\boldsymbol{r} - \boldsymbol{x}) \hat{W}_\varsigma),$$

where $\hat{W}_\varsigma$ satisfies Heisenberg's equation

$$i\hbar \dot{\hat{W}}_\varsigma = [\hat{H}(\hat{\boldsymbol{p}}, \hat{\boldsymbol{q}}), \hat{W}_\varsigma].$$

Let be $\hat{W}_\varsigma = \hat{W}_{0\varsigma} + \hat{W}_{1\varsigma}$, with $\hat{W}_{0\varsigma}$ as statistical operator for the thermodynamical equilibrium and define the trace with the help of Ψ_Q:

$$\begin{aligned}
u_\varsigma(\boldsymbol{x}, t) &= \sum_Q \int_{\Omega_N} \bar{\Psi}_Q(\boldsymbol{r}) \delta(\boldsymbol{r} - \boldsymbol{x}) \hat{W}_\varsigma \Psi_Q(\boldsymbol{r}) d\boldsymbol{r} \\
&= \sum_Q \bar{\Psi}_Q(\boldsymbol{x}) \hat{W}_\varsigma \Psi_Q(\boldsymbol{x}).
\end{aligned}$$

Note

$$\hat{W}_{0\varsigma} \Psi_Q(\boldsymbol{x}) = \mathcal{F}_\varsigma(\mathcal{E}_Q) \Psi_Q(\boldsymbol{x})$$

where

$$\mathcal{F}_\varsigma(\mathcal{E}_Q) = \frac{1}{1+\exp\left(-e_\varsigma \frac{\mathcal{E}_Q - \mathcal{E}_{F,\varsigma}}{k_B T}\right)}$$

is the Fermi-Dirac statistics. In device modelling it is common to ignore $\hat{W}_{1\varsigma}$ and to supply the Fermi-Dirac statistics with quasi Fermi potentials thus getting

$$u_\varsigma(\boldsymbol{x}) = \sum_Q \mathcal{F}_\varsigma(\mathcal{E}_Q)\bar{\Psi}_Q(\boldsymbol{x})\Psi_Q(\boldsymbol{x}).$$

To evaluate this formula one introduces the electronic density of states

$$\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}) := \sum_Q \delta(\tilde{\mathcal{E}} - \mathcal{E}_Q)\bar{\Psi}_Q(\boldsymbol{x})\Psi_Q(\boldsymbol{x})$$

and finds

$$\begin{aligned} u_\varsigma(\boldsymbol{x}) &= \int \mathcal{F}_\varsigma(\tilde{\mathcal{E}})\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x})\ d\tilde{\mathcal{E}} \\ &= \sum_Q \left[\int \mathcal{F}_\varsigma(\tilde{\mathcal{E}})\delta(\tilde{\mathcal{E}} - \mathcal{E}_Q) d\tilde{\mathcal{E}}\right] \bar{\Psi}_Q(\boldsymbol{x})\Psi_Q(\boldsymbol{x}). \end{aligned} \tag{A.4}$$

Being interested only in $\boldsymbol{x}_{(1)}$-dependent phenomena on the length scale of $L_1, \dots, L_d$ one assumes an averaging over a fundamental cell of the translation lattice of the bulk material and gets rid of the spatial dependency of the Bloch function $u_{\boldsymbol{k}_0\varsigma}(\boldsymbol{x})$. From (A.1) and (A.2) follows

$$\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)}) := \sum_Q \delta(\tilde{\mathcal{E}} - \mathcal{E}_Q)\bar{\psi}_{Q_{(1)}}(\boldsymbol{x}_{(1)})\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)}) \tag{A.5}$$

and finally

$$u_\varsigma(\mathcal{E}_{F,\varsigma}, \boldsymbol{x}_{(1)}) = \int \mathcal{F}_\varsigma(\tilde{\mathcal{E}})\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)})\ d\tilde{\mathcal{E}}. \tag{A.6}$$

In order to calculate $\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)})$ one transforms the $\boldsymbol{k}$–sum into a $\boldsymbol{k}$–integral [10, S. 36]:

$$\sum_{\boldsymbol{k}\in\mathbb{R}^{g-n}} \longrightarrow \frac{2\left(\prod_{j=d+1}^n L_j\right)}{(2\pi)^{n-d}} \int_{-\infty}^{\infty} dk_{d+1} \dots dk_n.$$

There is a factor 2 for spin degeneracy and one has to compute the following density of states:

$$\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)}) = \frac{2\left(\prod_{j=d+1}^n L_j\right)}{(2\pi)^{n-d}} \sum_{Q_{(1)}} \int_{-\infty}^{\infty} dk_{d+1} \dots dk_n\ \delta(\tilde{\mathcal{E}} - \mathcal{E}'(Q_{(1)}, \boldsymbol{k}_{(2)})) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2. \tag{A.7}$$

Let A be an orthogonal matrix ($A\,{}^tA = \mathbb{1}_{n-d}$) such that

$${}^tA(\boldsymbol{w}_{(2,2)} - \boldsymbol{w}_{(2,1)}\boldsymbol{w}_{(1,1)}^{-1}\boldsymbol{w}_{(1,2)})A = \operatorname{diag}\left(\frac{1}{m'_{d+1}}, \dots, \frac{1}{m'_n}\right).$$

Such a diagonalization is possible since $\boldsymbol{w}$ is symmetric: ${}^t\boldsymbol{w} = \boldsymbol{w}$ and is a result of the variable transformation $\boldsymbol{k}_{(2)} = A\boldsymbol{k'}_{(2)}$. The energy (A.3) has now the form

$$\mathcal{E}'_Q = \mathcal{E}'(Q_{(1)}, \boldsymbol{k'}_{(2)}) = -E_\varsigma(0) + \mathcal{E}_{Q_{(1)}} - e_\varsigma \frac{\hbar^2}{2} {}^t\boldsymbol{k'}_{(2)} \begin{pmatrix} \frac{1}{m'_{d+1}} & 0 & \dots & 0 \\ 0 & \frac{1}{m'_{d+2}} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \frac{1}{m'_n} \end{pmatrix} \boldsymbol{k'}_{(2)}$$

with strictly positive masses $m'_{d+1}, \dots, m'_n$. The integral is computed in generalized spherical coordinates

$$\begin{aligned} k'_{d+1} &= r\sqrt{m'_{d+1}} \sin\phi_{n-d-1} \dots \sin\phi_2 \sin\phi_1 \\ k'_{d+2} &= r\sqrt{m'_{d+2}} \sin\phi_{n-d-1} \dots \sin\phi_2 \cos\phi_1 \\ &\vdots \\ k'_{n-1} &= r\sqrt{m'_{n-1}} \sin\phi_{n-d-1} \cos\phi_{n-d-2} \\ k'_n &= r\sqrt{m'_n} \cos\phi_{n-d-1} \end{aligned}$$

with $0 \le r < \infty,\ 0 \le \phi_1 < 2\pi,\ 0 \le \phi_l < \pi\ \forall l \in [2, n-d-1]$

$$\begin{aligned} dk_{d+1} dk_{d+2} \dots dk_n &= (\det A) dk'_{d+1} dk'_{d+2} \dots dk'_n \\ &= (\det A) r^{n-d-1} \left(\prod_{j=d+1}^{n} \sqrt{m'_j} \right) dr\, dS_{n-d-1}, \end{aligned}$$

where dS_{n-d-1} denotes the surface element of the $(n-d-1)$–dimensional unit sphere in $\mathbb{R}^{n-d}$. With [43, S. 432]

$$\int dS_{n-d-1} = \frac{2\pi^{(n-d)/2}}{\Gamma\left(\frac{n-d}{2}\right)} =: S_{n-d-1} \tag{A.8}$$

and

$$\frac{2}{\hbar^2}\left(\mathcal{E}(Q_{(1)}, \boldsymbol{k'}_{(2)}) + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}}\right) = -e_\varsigma r^2$$

follows

$$dr = \frac{-e_\varsigma d\mathcal{E}(Q_{(1)}, \boldsymbol{k'}_{(2)})}{\sqrt{-2\hbar^2 e_\varsigma \left(\mathcal{E}(Q_{(1)}, \boldsymbol{k'}_{(2)}) + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}}\right)}}$$

and

$$\begin{aligned} \mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)}) = \frac{2^{(n-d)/2}\left(\prod_{j=d+1}^{n} \sqrt{m'_j} L_j\right) S_{n-d-1}}{(2\pi\hbar)^{n-d}} (\det A) \cdot \\ \cdot \sum_{Q_{(1)}} \left(-e_\varsigma(\tilde{\mathcal{E}} + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}})\right)^{\frac{n-d}{2}-1} \cdot \\ \cdot\, \Theta\left(-e_\varsigma(\tilde{\mathcal{E}} + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}})\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 \qquad d < n. \end{aligned}$$

At last one has to regard that $E_\varsigma(0)$ has in general multiplicity $\iota \in \mathbb{N}$. With $\iota_S := \iota \det A$ one gets

(A.9)

$$\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)}) = \frac{2^{(n-d)/2}\iota_S \left(\prod_{j=d+1}^{n} \sqrt{m_j'} L_j\right) S_{n-d-1}}{(2\pi\hbar)^{n-d}} \sum_{Q_{(1)}} \left(-e_\varsigma(\tilde{\mathcal{E}} + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}})\right)^{\frac{n-d}{2}-1} \cdot$$
$$\cdot\, \Theta\left(-e_\varsigma(\tilde{\mathcal{E}} + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}})\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 \qquad d < n.$$

For $d = n$ the k'–integration ceases to apply and one has ad hoc

$$\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)}) = 2\iota_S \sum_{Q_{(1)}} \delta\left(\tilde{\mathcal{E}} + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}}\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 \qquad d = n. \tag{A.10}$$

The case $d = 0$ gives

$$\mathcal{D}(\tilde{\mathcal{E}}, \boldsymbol{x}_{(1)}) = \frac{2^{n/2}\iota_S \left(\prod_{j=1}^{n} \sqrt{m_j'} L_j\right) S_{n-1}}{(2\pi\hbar)^{n}} \left(-e_\varsigma(\tilde{\mathcal{E}} + E_\varsigma(0))\right)^{\frac{n}{2}-1} \Theta\left(-e_\varsigma(\tilde{\mathcal{E}} + E_\varsigma(0))\right).$$

Θ is the Heaviside function $\Theta(x) = 1$ for $x \geq 0$ und $\Theta(x) = 0$ for $x < 0$.

Computing the carrier densities one has temporary to distinguish between electrons ($e_\varsigma = -1$) and holes ($e_\varsigma = 1$). Substituting (A.9) in (A.6) yields for electrons

$$u_2(\mathcal{E}_{F,2}, \boldsymbol{x}_{(1)}) = \frac{2^{(n-d)/2}\iota_S \left(\prod_{j=d+1}^{n} \sqrt{m_j'} L_j\right) S_{n-d-1}}{(2\pi\hbar)^{n-d}} \cdot$$
$$\cdot \sum_{Q_{(1)}} \int_{\mathcal{E}_{Q_{(1)}} - E_2(0)}^{\infty} \frac{\left(\mathcal{E} + E_2(0) - \mathcal{E}_{Q_{(1)}}\right)^{(n-d)/2-1}}{1 + \exp\left(\frac{\mathcal{E} - \mathcal{E}_{F,2}}{k_B T}\right)} \, d\mathcal{E} \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2$$

resp. for holes

$$u_1(\mathcal{E}_{F,1}, \boldsymbol{x}_{(1)}) = \frac{2^{(n-d)/2}\iota_S \left(\prod_{j=d+1}^{n} \sqrt{m_j'} L_j\right) S_{n-d-1}}{(2\pi\hbar)^{n-d}} \cdot$$
$$\cdot \sum_{Q_{(1)}} \int_{-\infty}^{\mathcal{E}_{Q_{(1)}} - E_1(0)} \frac{\left(-(\mathcal{E} + E_1(0) - \mathcal{E}_{Q_{(1)}})\right)^{(n-d)/2-1}}{1 + \exp\left(-\frac{\mathcal{E} - \mathcal{E}_{F,1}}{k_B T}\right)} \, d\mathcal{E} \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2.$$

The transformation ($T > 0\ K$)

$$\xi k_B T = -e_\varsigma(\mathcal{E} + E_\varsigma(0) - \mathcal{E}_{Q_{(1)}})$$
$$d\mathcal{E} = -e_\varsigma k_B T d\xi$$

leads to

$$u_\varsigma(\mathcal{E}_{F,\varsigma}, \boldsymbol{x}_{(1)}) = \frac{(2k_B T)^{(n-d)/2}\iota_S \left(\prod_{j=d+1}^{n} \sqrt{m_j'} L_j\right) S_{n-d-1}}{(2\pi\hbar)^{n-d}} \cdot$$
$$\cdot \sum_{Q_{(1)}} \int_0^{\infty} \frac{\xi^{(n-d)/2-1}}{1 + \exp\left(\xi + e_\varsigma \frac{E_\varsigma(0) + \mathcal{E}_{F,\varsigma} - \mathcal{E}_{Q_{(1)}}}{k_B T}\right)} \, d\xi \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2.$$

Using the definition of the Fermi integrals (cf. (1.4))

$$\mathfrak{F}_\alpha(\zeta) := \frac{1}{\Gamma(1+\alpha)} \int_0^\infty \frac{\xi^\alpha}{1+\exp(\xi-\zeta)}\, d\xi$$

one obtains for $d < n$:

$$u_\varsigma(\mathcal{E}_{F,\varsigma}, \boldsymbol{x}_{(1)}) = \frac{(2k_BT)^{(n-d)/2}\iota_S \left(\prod_{j=d+1}^n \sqrt{m_j'} L_j\right) S_{n-d-1}}{(2\pi\hbar)^{n-d}} \Gamma\left(\frac{n-d}{2}\right) \cdot \sum_{Q_{(1)}} \mathfrak{F}_{\frac{n-d}{2}-1}\left(-e_\varsigma \frac{E_\varsigma(0) + \mathcal{E}_{F,\varsigma} - \mathcal{E}_{Q_{(1)}}}{k_BT}\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 . \tag{A.11}$$

In the case of $d = n$ the density of states (A.10) is a sum of δ–functionals by itself and the integration is trivial:

$$\begin{aligned} u_\varsigma(\mathcal{E}_{F,\varsigma}, \boldsymbol{x}_{(1)}) &= 2\iota_S \sum_{Q_{(1)}} \frac{\left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2}{1+\exp\left(e_\varsigma \frac{E_\varsigma(0)+\mathcal{E}_{F,\varsigma}-\mathcal{E}_{Q_{(1)}}}{k_BT}\right)} \\ &= 2\iota_S \sum_{Q_{(1)}} \mathfrak{F}_{-1}\left(-e_\varsigma \frac{E_\varsigma(0)+\mathcal{E}_{F,\varsigma}-\mathcal{E}_{Q_{(1)}}}{k_BT}\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 . \end{aligned}$$

Two special cases are of interest:

(i) $d = 2,\ n = 3,\ T > 0$ K

Note that following (A.8) one has $S_0 = 2,\ S_1 = 2\pi,\ S_2 = 4\pi$. The result $S_0 = 2$ accounts correctly for the fact that a spherical symmetrical function over $\mathbb{R}$ is an even function. From (A.11) follows (cf. (1.15))

$$u_\varsigma(\mathcal{E}_{F,\varsigma}, \boldsymbol{x}_{(1)}) = 2\iota_S \sqrt{\frac{k_BTm_3'}{2\pi\hbar^2}}\, L_3 \sum_{Q_{(1)}} \mathfrak{F}_{-\frac{1}{2}}\left(-e_\varsigma \frac{E_\varsigma(0)+\mathcal{E}_{F,\varsigma}-\mathcal{E}_{Q_{(1)}}}{k_BT}\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 .$$

(ii) $d = 1,\ n = 3,\ T > 0$ K

Here from (A.11) follows (cf. (1.16))

$$u_\varsigma(\mathcal{E}_{F,\varsigma}, \boldsymbol{x}_{(1)}) = \iota_S \sqrt{m_2'm_3'}\, L_2L_3 \frac{k_BT}{\pi\hbar^2} \cdot \sum_{Q_{(1)}} \ln\left(1+\exp\left(-e_\varsigma \frac{\mathcal{E}_{F,\varsigma}+E_\varsigma(0)-\mathcal{E}_{Q_{(1)}}}{k_BT}\right)\right) \left|\psi_{Q_{(1)}}(\boldsymbol{x}_{(1)})\right|^2 .$$

$\mathbb{N}$	natural numbers
$\mathbb{R}$	real numbers
$\mathbb{C}$	complex numbers numbers
$X, Y, \ldots$	Banach spaces over $\mathbb{R}$ or $\mathbb{C}$
$X^*, Y^*, \ldots$	dual spaces to $X, Y, \ldots$
X^d	set of ordered d–tuples of elements from X
$T : X \mapsto Y$	operator from X into Y
$T^* : Y^* \mapsto X^*$	adjoint of a linear operator $T : X \mapsto Y$
	in particular conjugate of a complex number $T \in \mathbb{C}$
$\mathbb{1} : X \hookrightarrow Y$	(bounded) embedding operator from X into Y
$\\|\mathbb{1}\\|_{\mathcal{B}(X,Y)}$	embedding constant from X into Y
$\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_{[X^*,X]}$	dual pairing between the Banach space X and its dual X^*
$\langle \cdot, \cdot \rangle = \langle \cdot, \cdot \rangle_X$	scalar product in the Hilbert space X
$\\| \cdot \\|_X$	norm in the Banach space X
$\mathcal{B}(X, Y)$	space of bounded linear operators from X into Y
$\mathcal{B} = \mathcal{B}(X, Y)$	usually with $X = Y = L^2(\Omega)$
$\\| \cdot \\| = \\| \cdot \\|_{\mathcal{B}(X,Y)}$	usually with $X = Y = L^2(\Omega)$
$\mathcal{B}_q(X, Y)$	space of q–summable operators from X into Y
$\mathcal{B}_q = \mathcal{B}_q(X, Y)$	usually with $X = Y = L^2(\Omega)$
$\\| \cdot \\|_q = \\| \cdot \\|_{\mathcal{B}_q(X,Y)}$	usually with $X = Y = L^2(\Omega)$
$\Omega, \hat{\Omega}, \tilde{\Omega}$	bounded open subsets of $\mathbb{R}^d$
$\partial\Omega$	boundary of Ω
$L^\infty(\Omega, X)$	space of all essentially bounded Lebesgue–measurable functions from Ω into a Banach space X
$L^\infty(\Omega) = L^\infty(\Omega, \mathbb{R})$	
$L^p(\Omega, X)$, $1 \le p < \infty$	space of p–integrable functions
$L^p(\Omega) = L^p(\Omega, \mathbb{R})$	
$W^{1,p}(\Omega)$	Sobolev space with the usual norm $\\|u\\|_{W^{1,p}(\Omega)} = \left(\\|u\\|^p_{L^p(\Omega)} + \\|\operatorname{grad} u\\|^p_{L^p(\Omega)}\right)^{\frac{1}{p}}$
$\operatorname{dom}(T)$	domain of the linear operator T
$\operatorname{spec}[T]$	spectrum of the linear operator T
$\operatorname{tr}[T]$	trace of the nuclear operator T
$\operatorname{sp}(\phi)$	trace of the function $\phi : \Omega \mapsto \mathbb{R}$ on the boundary $\partial\Omega$
$\operatorname{grad} u$	gradient of $u \in L^p(\Omega)$
$\operatorname{div} f$	divergence of $f \in L^p(\Omega, \mathbb{R}^d)$
$C^\alpha(\Omega, X)$, $0 < \alpha < 1$	space of all functions from Ω into X that are Hölder continuous with exponent α
$C^\alpha(\Omega) = C^\alpha(\Omega, \mathbb{R})$	
$C^l(\overline{\Omega}, X)$	space of all functions from $\overline{\Omega}$ into X with continuous derivatives up to order l
$C^l(\overline{\Omega}) = C^l(\overline{\Omega}, \mathbb{R})$	
$C(\overline{\Omega}, X)$	space of all continuous functions from $\overline{\Omega}$ into X
$C(\overline{\Omega}) = C(\overline{\Omega}, \mathbb{R})$	

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