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On Stationary Schrödinger–Poisson Equations

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On Stationary Schrödinger–Poisson Equations Modelling an Electron Gas with Reduced Dimension (by H.–Chr. Kaiser and J. Rehberg)

Abstract: We regard the Schrödinger–Poisson system arising from the modelling of an electron gas with reduced dimension in a bounded up to three–dimensional domain and establish the method of steepest descent. The electrostatic potentials of the iteration scheme will converge uniformly on the spatial domain. To get this result we investigate the Schrödinger operator, the Fermi level and the quantum mechanical electron density operator for square integrable electrostatic potentials. On bounded sets of potentials the Fermi level is continuous and bounded, and the electron density operator is monotone and Lipschitz continuous. — As a tool we develop a Riesz–Dunford functional calculus for semibounded self–adjoint operators using paths of integration which enclose a real half axis.

Key words: stationary Schrödinger–Poisson system, monotone potential operators, iterative methods, electron gas with reduced dimension, nanoelectronics.

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1. The Schrödinger–Poisson Equation

The Schrödinger–Poisson system is a nonlinear Poisson equation

$$-\Delta V = n(V_0 + V) - n_D \quad \text{in } \Omega, \quad V|_{\partial\Omega} = 0 \tag{1.1}$$

for the electrostatic potential V, the right–hand side of which is up to a fixed part n_D the quantum mechanical expression of the electron density

$$n(V_0 + V)(x) = \sum_{l=1}^{\infty} f(\epsilon_l - \epsilon_0)|\psi_l(x)|^2, \quad x \in \Omega, \tag{1.2}$$

where $\epsilon_l = \epsilon_l(V_0 + V)$ are the eigenvalues (in increasing order, counting multiplicity) and $\psi_l = \psi_l(V_0 + V)$ the corresponding orthonormal eigenfunctions of the Schrödinger equation

$$(-\Delta + V_0 + V)\psi_l = \epsilon_l\psi_l \quad \text{in } \Omega, \quad \psi_l|_{\partial\Omega} = 0, \quad \int_\Omega |\psi_l|^2 = 1, \quad l = 1, 2, \ldots . \tag{1.3}$$

$V_0 \in L^2(\Omega; \mathbf{R})$ is a given external potential and $\epsilon_0 = \epsilon_0(V_0 + V)$ denotes the Fermi level which is defined by the electric–neutrality condition

$$\int_\Omega n_D(x)dx = \int_\Omega n(V_0 + V)(x)dx = \sum_{l=1}^{\infty} f(\epsilon_l(V_0 + V) - \epsilon_0(V_0 + V)), \tag{1.4}$$

f being the thermodynamical equilibrium distribution function. Thus, ϵ_0 in general depends on the potential in the Schrödinger equation. We will also regard the auxiliary problem (1.1)–(1.3), where ϵ_0 is a given parameter. The Schrödinger–Poisson system (1.1)–(1.4) models an electron gas with reduced dimension situated in the bounded spatial domain $\Omega \subset \mathbf{R}^d$, $d \leq 3$ (cf. Albinus in this preprint, [2] and the references cited there). For a zero–, one– or two–dimensional electron gas the dimension d of the spatial domain Ω is $d = 3, 2, 1$, respectively. N.B. we make use of the assumption $d \leq 3$ without further notice throughout this paper which comes to bear especially when Sobolev's Embedding Theorem is involved.

The Schrödinger–Poisson system can be written as a nonlinear operator equation

$$A(V) = -n_D, \quad V \in H_0^1(\Omega; \mathbf{R}) \tag{1.5}$$

in the Sobolev space $H^{-1}(\Omega;\mathbf{R})$. The Schrödinger–Poisson operator $A \in (H_0^1 \to H^{-1})$ is defined by

$$\langle A(V)\,,\,W\rangle := \int_\Omega (\nabla W\cdot\nabla V - Wn(V_0+V))dx, \quad \forall V,W\in H_0^1(\Omega;\mathbf{R}), \qquad (1.6)$$

i.e. it is the difference of the duality mapping $J\in\mathcal{B}(H_0^1,H^{-1})$ of the space $H_0^1(\Omega;\mathbf{R})$ equipped with the norm $\|u\|_{H_0^1} = \|\nabla u\|_{L^2}$ and the electron–density operator n which maps $L^2(\Omega;\mathbf{R})$ into $L^\infty(\Omega;\mathbf{R})$ (cf. §6.1). The operator equation (1.5) makes sense if $n_D \in H^{-1}(\Omega;\mathbf{R})$. On the other hand we need $n_D\in L^1(\Omega;\mathbf{R})$ in order to formulate the electric–neutrality condition (1.4). To cover both demands we assume $n_D\in L^2(\Omega;\mathbf{R})$.
Recently NIER showed [10], [11] that the Schrödinger–Poisson operator (1.6) is a strongly monotone potential operator. To that end he regarded the functional

$$\phi(U) = \epsilon_0(U)\ \mathrm{tr}\,(f(H_U-\epsilon_0(U))) + \mathrm{tr}\,(F(H_U-\epsilon_0(U)))\,. \qquad (1.7)$$

for electrostatic potentials $U = V_0+V$ from the affine space $V_0 + H_0^1(\Omega;\mathbf{R})$. In (1.7) $H_U = -\Delta + V_0 + V \in (L^2(\Omega)\to L^2(\Omega))$ is the Schrödinger operator with domain $H^2(\Omega)\cap H_0^1(\Omega)$ and F is the primitive

$$F(t) = -\int_t^\infty f(s)ds, \quad t\in\mathbf{R} \qquad (1.8)$$

of the distribution function f. ϕ is infinitely often Fréchet differentiable and the first derivative of ϕ is just the electron density which turns out to be a strictly monotone operator $n\in(V_0+H_0^1(\Omega;\mathbf{R})\to H^{-1}(\Omega;\mathbf{R}))$. Thus, the operator equation (1.5) is equivalent to the minimization problem

$$\mathcal{I}(V) = \min_{W\in H_0^1}\mathcal{I}(W), \quad \mathcal{I}(W) := \frac{1}{2}\|W\|_{H_0^1} - \phi(V_0+W) + \langle n_D, W\rangle. \qquad (1.9)$$

We will regard the functional (1.7) on the space $L^2(\Omega;\mathbf{R})$. In order to get the Fréchet differentiability of ϕ and n on that space we will prove

i. the uniform equivalence of the graph–norms belonging to Schrödinger operators with potentials from any bounded set in $L^2(\Omega;\mathbf{R})$ (cf. §3.4),
ii. the boundedness of the Fermi level on every L^2–bounded set of electrostatic potentials (cf. §5).

We also prove that the electron–density operator n is monotone and bounded Lipschitzian as an operator $n\in(L^2(\Omega;\mathbf{R})\to L^2(\Omega;\mathbf{R}))$. This guarantees the convergence of the method of steepest descent applied to the Schrödinger–Poisson equation (1.5) and allows to establish even uniform convergence on Ω for the iteration sequence of electrostatic potentials. Thus we can estimate the distance of the spectra and even of single eigenvalues of the Schrödinger operators corresponding to the potentials from the iteration sequence, using eigenvalue perturbation theory [17], [9], [14].
NIER [11] operates with a functional calculus for self–adjoint operators due to HELFFER, SJÖSTRAND and GÉRARD. We develop a Riesz–Dunford calculus instead (cf. §4) which in principle allows an extension to m–accretive operators. One has to cope with Schrödinger operators of this kind when a magnetic field is included in the problem, or when other boundary conditions are regarded.

When dealing with the Schrödinger–Poisson equation we operate with spaces of real–valued functions whereas the Schrödinger operator is defined on a space of complex–valued functions. N.B. we regard solely real–valued potentials for the Schrödinger operator. In the sequel we will use the same notation for spaces of complex–valued functions and the corresponding subspaces of real valued functions.

Throughout this paper we make the following assumptions about the data of the problem:

• The spatial domain $\Omega \subset \mathbf{R}^d$, $(d \leq 3)$ in which we regard the Schrödinger–Poisson system is assumed to be in the GRÖGER–class $\mathfrak{R}_{p_0}$ (cf. [5]) for some $p_0 > d$, i.e. Ω is regular in the sense of GRÖGER (e.g. bounded and open) and the duality mapping

$$J \in \left(H_0^1(\Omega) \to H^{-1}(\Omega)\right) \quad \langle Ju, v\rangle = \int_\Omega \nabla v \cdot \nabla \bar{u} dx \quad u, v \in H_0^1(\Omega) \tag{1.10}$$

of the Sobolev space $H_0^1(\Omega)$ maps $W_0^{1,p_0}(\Omega)$ **onto** $W^{-1,p_0}(\Omega)$. Thus, the operator

$$J_p = J|_{W_0^{1,p}} \in \left(W_0^{1,p}(\Omega) \to W^{-1,p}(\Omega)\right) \tag{1.11}$$

is a continuous bijection for all $2 \leq p \leq p_0$ (cf. [5]). A theorem of GRÖGER and REHBERG [6] then gives that the mapping

$$J_p + \lambda I \in \left(W_0^{1,p}(\Omega) \to W^{-1,p}(\Omega)\right) \tag{1.12}$$

is a continuous bijection from $W_0^{1,p}$ onto $W^{-1,p}$ for all $\lambda \in C$ with $\Re\lambda \geq 0$. Hence the adjoint of the linear operator (1.12)

$$\left((J_p + \lambda I)|_{W_0^{1,p}}\right)^* \in \left(W_0^{1,q}(\Omega) \to W^{-1,q}(\Omega)\right), \quad 1/p + 1/q = 1$$

is a continuous bijection from $W_0^{1,q} = (W^{-1,p})^*$ onto $W^{-1,q} = \left(W_0^{1,p}\right)^*$. There is for all $u \in W_0^{1,p}$ and $v \in W_0^{1,q}$

$$\langle u, (J_p + \lambda I)^* v\rangle = \langle (J_p + \lambda I)u, v\rangle = \langle (J + \lambda I)u, v\rangle = \int_\Omega (\lambda v\bar{u} + \nabla v \cdot \nabla \bar{u})\, dx,$$

i.e. $(J_p + \lambda I)^*$ is the extension $J_q + \lambda I$ of the operator $J + \lambda I \in \mathcal{B}\left(W_0^{1,2}, W^{-1,2}\right)$, to the space $W_0^{1,q}$. Thus,

$$J_p + \lambda I \in \mathcal{B}\left(W_0^{1,p}, W^{-1,p}\right) \qquad \Re\lambda \geq 0 \qquad \frac{p_0}{p_0 - 1} \leq p \leq p_0 \tag{1.13}$$

is a continuous bijection.

For any Lipschitz–domain Ω there is a $p_0 > 2$ such that $\Omega \in \mathfrak{R}_{p_0}$ [5]. This suffices in the two–dimensional case $(d = 2)$. In general, as we regard homogeneous Dirichlet boundary conditions, $\Omega \in \mathfrak{R}_p$ is satisfied for all $2 \leq p < \infty$ if Ω is a bounded domain of class C^1 (cf. [16]). Furthermore we assume Ω to be such that J maps the space $H^2(\Omega) \cap H_0^1(\Omega)$ **onto** $L^2(\Omega)$, i.e. the Laplacian

$$-\Delta = J|_{H^2 \cap H_0^1} \in \left(H^2(\Omega) \cap H_0^1(\Omega) \to L^2(\Omega)\right) \tag{1.14}$$

is a continuous bijection. This hypothesis is satisfied if Ω is a bounded domain of class C^2 or convex polygonal (cf. [4] and the references cited there).

• The given external potential V_0 is assumed to be real–valued and square integrable on Ω. It represents the electronic characteristics of the material, the positive background charge, the applied voltage and eventually inhomogeneous boundary conditions for the potential.

• The fixed part n_D on the right–hand side of the nonlinear Poisson equation also shall be a square integrable function on Ω. It stands for a given density of ionized impurities.

• The thermodynamical equilibrium distribution function f defines the occupation factor $N_l = f(\epsilon_l - \epsilon_0)$ which is the average number of electrons in the quantum state l with the energy ϵ_l at thermodynamical equilibrium. f is assumed to be positive and strictly decreasing and the primitive (1.8) should exist. We will further specify f in §4.2.

2. The Schrödinger operator

2.1. The Dirichlet–problem for the Laplacian. According to the assumptions about the regularity of the spatial domain Ω the Laplacian with homogeneous Dirichlet–boundary–conditions (cf. (1.14)) has the following properties:

- $-\Delta$ is a self–adjoint, positive definite operator with compact resolvent in the Hilbert space $L^2(\Omega)$.
- The spectrum of $-\Delta$ is discrete; there is a countable number of real eigenvalues λ_l (counting multiplicity)

$$0 < m = \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots\,, \qquad \lambda_l \to \infty$$

  and eigenfunctions ψ_l spanning an orthonormal basis in $L^2(\Omega)$; the asymptotical distribution of the eigenvalues is [18], [14]

$$\lim_{l\to\infty} \frac{l^2}{\lambda_l^d} = c\,|\Omega|^2. \tag{2.1}$$

- The H^2–norm, the graph norm of $-\Delta$ and $\|(\rho-\Delta)\cdot\|_{L^2}$, $\rho > 0$ are equivalent on $\operatorname{dom}\Delta = H^2(\Omega)\cap H_0^1(\Omega)$

$$\|\cdot\|_{H^2(\Omega)} \sim \|(i-\Delta)\cdot\|_{L^2(\Omega)} \sim \|(\rho-\Delta)\cdot\|_{L^2(\Omega)} \quad \forall \rho > 0. \tag{2.2}$$

Proposition 2.1. *Let be $\rho > 0$ and $0 \leq \theta < 1/2$. The operator $(\rho-\Delta)^{1-\theta}$ is a continuous bijection of $H^{2(1-\theta)}(\Omega)\cap H_0^{1-\theta}(\Omega)$* **onto** *$L^2(\Omega)$.*

Proof. The operator $\rho - \Delta$ is self–adjoint and positive definite in L^2, and its domain $H^2 \cap H_0^1$ is a Hilbert space $(\operatorname{dom}(\rho-\Delta), \|(\rho-\Delta)\cdot\|_{L^2})$ which is dense in L^2. Hence the interpolation space

$$\operatorname{dom}(\rho-\Delta)^{1-\theta} = \left[\operatorname{dom}(\rho-\Delta), L^2\right]_\theta = \left[H^2, L^2\right]_\theta \cap \left[H_0^1, L^2\right]_\theta = H^{2(1-\theta)} \cap H_0^{1-\theta}$$

becomes a Hilbert space with the graph norm of $(\rho-\Delta)^{1-\theta}$ [8]. Moreover, the graph norm of $(\rho-\Delta)^{1-\theta}$ and the norm of $H^{2(1-\theta)} \cap H_0^{1-\theta}$ are equivalent. Thus, $(\rho-\Delta)^{1-\theta} \in \mathcal{B}\left(H^{2(1-\theta)} \cap H_0^{1-\theta}, L^2\right)$. As $t^{1-\theta}$ maps $\mathbf{R}^+$ one–to–one onto $\mathbf{R}^+$, $(\rho-\Delta)^{1-\theta}$ is a bijection because $(\rho-\Delta)$ is. $\square$

2.2. Self–adjointness, lower bound and spectrum. We regard the Schrödinger operator

$$H = H_V = -\Delta + V \in \left(L^2(\Omega) \to L^2(\Omega)\right), \quad \operatorname{dom} H = H^2(\Omega) \cap H_0^1(\Omega) \qquad (2.3)$$

for real–valued potentials $V \in L^2(\Omega)$ and recall (cf. [11])

Proposition 2.2. *For each $V \in L^2(\Omega)$ the multiplication operator $V \in (L^2 \to L^2)$ is infinitesimally small with respect to $-\Delta$ i. e. the relative $-\Delta$-bound of V is zero:*

$$\|V\psi\|_{L^2} \leq \delta \|\Delta\psi\|_{L^2} + C\|\psi\|_{L^2}, \quad \forall \psi \in H^2(\Omega), \quad \forall \delta > 0$$

with some $C = C(\delta, \|V\|_{L^2})$.

As V is real–valued, the multiplication operator $V \in (L^2 \to L^2)$ is self–adjoint on $\operatorname{dom} V = \{\psi \in L^2(\Omega) \,:\, V\psi \in L^2(\Omega)\}$ and by Sobolev's Embedding Theorem

$$\operatorname{dom} \Delta \subset H^2(\Omega) \hookrightarrow L^\infty(\Omega) \subset \operatorname{dom} V.$$

Thus, by the Kato–Rellich Theorem H is self–adjoint. The multiplication operator V is also relatively compact with respect to $-\Delta$, because the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ is compact. Hence, by Weyl's Theorem the essential spectrum of H and $-\Delta$ is the same and we conclude that the spectrum of the Schrödinger operator (2.3) is discrete i.e. H_V has a countable number of real eigenvalues $\{\epsilon_l(V)\}_{l=1}^{\infty}$ (counting multiplicity) and the corresponding orthonormal eigenfunctions provide a basis of $L^2(\Omega)$.

Proposition 2.3. *For each (real–valued) potential $V \in L^2(\Omega)$ the graph–norms of the Schrödinger operator* (2.3) *and the Laplacian* (1.14) *are equivalent:*

$$C(V)\|(i-\Delta)\psi\|_{L^2} \leq \|(H+i)\psi\|_{L^2} \leq \tilde{C}(V)\|(i-\Delta)\psi\|_{L^2}, \quad \forall \psi \in \operatorname{dom} H.$$

Proof. As H and $-\Delta$ are self–adjoint their domain $\operatorname{dom} H = \operatorname{dom} \Delta$ becomes a Banach space

$$\mathfrak{B}_H = (\operatorname{dom} H,\ \|(H+i)\cdot\|_{L^2}) \quad \mathfrak{B}_\Delta = (\operatorname{dom} H,\ \|(i-\Delta)\cdot\|_{L^2})$$

with the corresponding graph norm. As the embedding $H^2 \hookrightarrow L^\infty$ is continuous and according to (2.2) there is by Proposition 2.2

$$\|V\psi\|_{L^2} \;\leq\; \|V\|_{L^2}\|\psi\|_{L^\infty} \;\leq\; c_0\|V\|_{L^2}\|\psi\|_{H^2} \;\leq\; c\,\|V\|_{L^2}\|(i-\Delta)\psi\|_{L^2}$$

and we may notice

$$\|(H+i)\psi\|_{L^2} \leq (1 + c\|V\|_{L^2})\ \|(i-\Delta)\psi\|_{L^2}, \quad \forall \psi \in \operatorname{dom} H,$$

i.e. the embedding $\mathfrak{B}_\Delta \to \mathfrak{B}_H$ is bounded and as it is bijective too, so is its inverse by the Inverse Mapping Theorem. □

Corollary 2.1. *For every $\rho > \max\{0, -\epsilon_1(V)\}$ the norms $\|(\rho + H)\cdot\|_{L^2}$ and $\|(\rho - \Delta)\cdot\|_{L^2}$ are equivalent on* $\operatorname{dom} H = \operatorname{dom} \Delta = H^2(\Omega) \cap H_0^1(\Omega)$.

Theorem 2.1. *Let be $M > 0$ arbitrary and $\mathcal{M}$ the closed M–ball of $L^2(\Omega)$. Then the infima $\epsilon_1(V)$ of the spectra from the Schrödinger operators $H_V = -\Delta + V$ corresponding to the potentials $V \in \mathcal{M}$ are bounded:*

$$-\infty < \sigma_M \leq \epsilon_1(V) \leq \Sigma_M < \infty, \qquad \forall V \in \mathcal{M}. \qquad (2.4)$$

Proof. We first show that the spectra are uniformly bounded from below. By a corollary of the Kato–Rellich Theorem H_V is bounded from below with

$$\sigma_V(\delta) = m - \max\left\{\frac{C\left(\delta, \|V\|_{L^2}\right)}{1-\delta}\ , \ \delta m + C\left(\delta, \|V\|_{L^2}\right)\right\}\ ,$$

for all $0 < \delta < 1$, where m is the smallest eigenvalue of $-\Delta$ and $C = C\left(\delta, \|V\|_{L^2}\right)$ is the constant from Proposition 2.2. Hence for all $V \in L^2$ with $\|V\|_{L^2} \leq M$ the spectrum $\sigma(H_V)$ of H_V is bounded from below by

$$\sigma_M = \sup_{0<\delta<1}\left\{m - \max\left\{\frac{C\left(\delta, M\right)}{1-\delta}, \delta m + C\left(\delta, M\right)\right\}\right\}. \tag{2.5}$$

Next we give an upper bound for the infima of the spectra. The smallest eigenvalue $\epsilon_1(V)$ of H_V is given by (N.B. $\operatorname{dom} H_V = \operatorname{dom}\Delta = H^2 \cap H_0^1$)

$$\epsilon_1(V) = \inf_{\substack{\psi\in\operatorname{dom}\Delta\\ \|\psi\|_{L^2}=1}} \langle(-\Delta + V)\psi, \psi\rangle.$$

For all $\psi \in \operatorname{dom}\Delta$ there is

$$\langle(-\Delta + V)\psi, \psi\rangle \leq \langle-\Delta\psi, \psi\rangle + \langle|V|\psi, \psi\rangle = \langle-\Delta\psi, \psi\rangle + \left\|\sqrt{|V|}\psi\right\|_{L^2}.$$

We estimate the second term on the right–hand side

$$\left\|\sqrt{|V|}\psi\right\|_{L^2} \leq \left\|\sqrt{|V|}\right\|_{L^4} \|\psi\|_{L^4} = \sqrt{\|V\|_{L^2}}\ \|\psi\|_{L^4} \leq \sqrt{M}\ \|\psi\|_{L^4}.$$

For all $\psi \in \operatorname{dom}\Delta$ there is

$$\|\psi\|_{L^4} \leq c_0\|\psi\|_{H_0^1} = c_0\|\nabla\psi\|_{L^2} = c_0\langle-\Delta\psi, \psi\rangle,$$

where c_0 is the embedding constant of $H_0^1(\Omega)$ into $L^4(\Omega)$. Putting together the above estimates one obtains

$$\epsilon_1(V)\ \leq\ \left(1 + c_0\sqrt{M}\right) \inf_{\substack{\psi\in\operatorname{dom}\Delta\\ \|\psi\|_{L^2}=1}} \langle-\Delta\psi, \psi\rangle = \left(1 + c_0\sqrt{M}\right) m, \tag{2.6}$$

where $m > 0$ is the smallest eigenvalue of $-\Delta$. $\square$

3. The resolvent of the Schrödinger operator

For a separable Hilbert space $\mathcal{H}$, later on unless specifically noticed $L^2(\Omega)$ let denote $\mathcal{B} = \mathcal{B}(\mathcal{H}) = \mathcal{B}(\mathcal{H}, \mathcal{H})$ the Banach algebra of bounded linear operators on $\mathcal{H}$ with the usual norm $\|\cdot\|$ for linear operators, $\mathcal{B}_0$ the subspace of finite rank operators, $\mathcal{B}_\infty$ the closed ideal of compact operators, $(\mathcal{B}_p, \|\cdot\|_p)$, $1 \leq p < \infty$ the closed ideal of p–summable operators . An operator $A \in \mathcal{B}_\infty$ with a discrete spectrum of eigenvalues $\alpha_1, \alpha_2, \ldots$ belongs to the summability–class $\mathcal{B}_p$ if the sequence $\{\alpha_l\}_{l=1}^\infty$ is p–summable: $\{\alpha_l\}_{l=1}^\infty \in l_p$ (cf. e.g. [15]).

3.1. The resolvent of the Laplacian. Let us regard again the homogeneous Dirichlet problem for the Laplacian. For all $z \in C$ with $\Re z \le 0$ the corresponding resolvent of the Laplacian (1.14) is compact

$$(\Delta + z)^{-1} \in \mathcal{B}_\infty, \quad \forall z \in C,\ \Re z \le 0 \tag{3.1}$$

and there is

$$\|(\Delta + z)^{-1}\| = \|(\Delta + z)^{-1}\|_\infty = \frac{1}{|z + \lambda_1|} \le \frac{1}{\lambda_1} < \infty.$$

In the same way one obtains

$$(\Delta + z)^{-\alpha} \in \mathcal{B}_\infty, \quad \forall z \in C,\ \Re z \le 0, \quad \forall \alpha > 0, \quad \|(\Delta + z)^{-\alpha}\| \le \frac{1}{\lambda_1^\alpha} < \infty. \tag{3.2}$$

Apart of compactness we even get p–summability (cf. [11]).

Lemma 3.1. *The resolvent $(\Delta + z)^{-1}$ belongs to the space $\mathcal{B}_p$ for any $p > d/2$ and all $z \in C$ with $\Re z \le 0$.*

Proof. Let be $0 < \lambda_1 \le \lambda_2 \le \ldots$ the eigenvalues of $-\Delta$ (counting multiplicity). Then the eigenvalues of the resolvent are $\frac{1}{z-\lambda_l}$, $l = 1, 2, \ldots$ and as

$$|z - \lambda_l| \ge |\Re z - \lambda_l| \ge \lambda_l$$

one gets

$$\|(\Delta + z)^{-1}\|_p^p = \sum_{l=1}^\infty \frac{1}{|z - \lambda_l|^p} \le \sum_{l=1}^\infty \frac{1}{\lambda_l^p}.$$

This series converges for any $p > d/2$ as $\sum_{l=1}^\infty (1/l)^{2p/d}$ according to (2.1). $\square$

Corollary 3.1. *For each $\alpha > 0$ there is*

$$(\Delta + z)^{-\alpha} \in \mathcal{B}_p \quad \forall z \in C,\ \Re z \le 0, \quad \forall p > d/(2\alpha). \tag{3.3}$$

As the summability–classes $\mathcal{B}_p$ are two–sided ideals in $\mathcal{B}$ the operators $(\Delta - \rho)^{-1}$ and $V(\Delta - \rho)^{-1}$ are from the same summability–class for all $V \in L^\infty(\Omega)$. Next we will have a look at the

3.2. Summability–class of the operators $V(\Delta - \rho)^{-1}, \rho > 0, V \in L^2(\Omega)$. For each $V \in L^2(\Omega)$ the mapping

$$\psi \in L^2 \to (\Delta - \rho)^{-1}\psi \in H^2 \to V(\Delta - \rho)^{-1}\psi \in L^2$$

is compact, because the embedding $H^2 \hookrightarrow L^\infty$ is compact, i. e. $V(\Delta - \rho)^{-1} \in \mathcal{B}_\infty$. We will prove $V(\Delta - \rho)^{-1} \in \mathcal{B}_p, \forall p > 2d$.

Lemma 3.2. *For all $\rho > 0$ and $p > 2d$ the linear mapping*

$$\mathcal{V} \in \left(L^2(\Omega) \to \mathcal{B}_p\right) \qquad \mathcal{V}(V) = V(\Delta - \rho)^{-1} \tag{3.4}$$

is (uniformly in ρ) continuous.

Proof. We decompose with $0 < \theta < 1/4$

$$V(\Delta - \rho)^{-1} = V(\Delta - \rho)^{\theta-1}(\Delta - \rho)^{-\theta}.$$

According to Corollary 3.1 we have $(\Delta - \rho)^{-\theta} \in \mathcal{B}_p, \forall p > d/(2\theta)$. Now by Proposition 2.1 there is for all $\psi \in L^2(\Omega)$

$$\begin{aligned}\|V(\Delta-\rho)^{\theta-1}\psi\|_{L^2} &\le \|V\|_{L^2}\|(\Delta-\rho)^{\theta-1}\psi\|_{L^\infty} \le c_0\|V\|_{L^2}\|(\Delta-\rho)^{\theta-1}\psi\|_{H^{2(1-\theta)}} \\ &\le c\,\|V\|_{L^2}\|\psi\|_{L^2}\end{aligned}$$

(N.B. the embedding $H^{2(1-\theta)} \hookrightarrow L^\infty$ is continuous as $2(1-\theta) > d/2$ and the $H^{2(1-\theta)}$–norm is the norm of $H^{2(1-\theta)} \cap H_0^{1-\theta}$). We conclude by assembling the estimates in the following way

$$\|V(\Delta-\rho)^{-1}\|_p \le \|V(\Delta-\rho)^{\theta-1}\|\;\|(\Delta-\rho)^{-\theta}\|_p \le c\|V\|_{L^2}.$$

There is a suitable $\theta < 1/4$ for every $p > 2d$ and the constant c depends on p but not on ρ. □

In the two–dimensional case for $V \in L^2(\Omega)$ the operator $(\Delta-\rho)^{-1}V(\Delta-\rho)^{-1}$ is nuclear, more precisely

Corollary 3.2. *For all* $1 \le p < \infty$ *with* $p > 2d/5$ *and each* $V \in L^2(\Omega)$ *there is* $(\Delta-\rho)^{-1}V(\Delta-\rho)^{-1} \in \mathcal{B}_p$ *if* $\rho > 0$, *and*

$$\|(\Delta-\rho)^{-1}V(\Delta-\rho)^{-1}\|_p \le c\|V\|_{L^2} \quad \forall \rho > 0.$$

Proof. By means of Hölder's inequality, Lemmata 3.1 and 3.2 one obtains

$$\|(\Delta-\rho)^{-1}V(\Delta-\rho)^{-1}\|_p \le \|(\Delta-\rho)^{-1}\|_{p_1}\,\|V(\Delta-\rho)^{-1}\|_{p_2} \le c\|V\|_{L^2}$$

where $1 \ge 1/p = 1/p_1 + 1/p_2$ and $p_1 > d/2$, $p_2 > 2d$ i.e. p is greater than $2d/5$. Thus, in the two–dimensional case (d=2) the operator $(\Delta-\rho)^{-1}V(\Delta-\rho)^{-1}$ is indeed nuclear. □

3.3. Calculations with resolvents. Let us regard the Schrödinger operators (2.3) $H_j = -\Delta + V_j$ corresponding to potentials $V_j \in L^2(\Omega)$, $j = 1, 2$ and their resolvents $R_j = R_j(z) = (z - H_j)^{-1}$ at a common regular point z. We can decompose the difference of these resolvents in the following way

$$\begin{aligned}R_2 - R_1 &= R_2(1 - R_2^{-1}R_1) = R_2(R_1^{-1}R_1 - R_2^{-1}R_1) \\ &= R_2(R_1^{-1} - R_2^{-1})R_1 = R_2\,(V_2 - V_1)\,R_1.\end{aligned}$$

Using this decomposition a second time one gets

$$R_2 - R_1 = R_1VR_1 + (R_2 - R_1)VR_1 = R_1VR_1 + R_2VR_1VR_1,$$

where $V = V_2 - V_1$. Continuing this way one obtains the expansion

$$R_2 = R_1\left(\sum_{l=0}^{L-1}(VR_1)^l\right) + R_2(VR_1)^L \quad \forall L = 1, 2, \ldots. \tag{3.5}$$

By means of (3.5) the difference of resolvent–squares can be decomposed as follows

$$\begin{aligned} R_2^2 - R_1^2 &= R_2(R_2 - R_1) + (R_2 - R_1)R_1 \\ &= R_1(R_2 - R_1) + (R_2 - R_1)R_1 + (R_2 - R_1)(R_2 - R_1) \\ &= R_1^2 V R_1 + R_1 V R_1^2 + R_1 R_2 (V R_1)^2 + R_2 (V R_1)^2 R_1 + (R_2 V R_1)^2. \end{aligned}$$

3.4. L^2–bounded sets of potentials. We regard the Schrödinger operators (2.3) corresponding to potentials V from the closed M–ball $\mathcal{M}$ in $L^2(\Omega)$ and denote the resolvent of H_V at $z = -\rho_M = \sigma_M - 1$ (cf. (2.5)) by

$$R_V = (-\rho_M - H_V)^{-1} = (\Delta - \rho_M - V)^{-1}. \tag{3.6}$$

According to Theorem 2.1 $z = -\rho_M$ is a common regular point for all the Schrödinger operators under consideration.

Theorem 3.1. *The norms $\|(H_V + \rho_M) \cdot \|_{L^2}$ related to the Schrödinger operators H_V, $V \in \mathcal{M}$ are uniformly equivalent, i.e. there is a constant C_M such that*

$$C_M \, \|(H_V + \rho_M)^{-1}(\rho_M - \Delta)\| \le 1, \quad \forall V \in \mathcal{M}.$$

Remark 3.1. As ρ_M is a real value there is

$$\left[(\rho_M - \Delta)(H_V + \rho_M)^{-1}\right]^* = (H_V + \rho_M)^{-1}(\rho_M - \Delta)$$

and we have for all potentials $V \in \mathcal{M}$

$$\|(\rho_M - \Delta)(H_V + \rho_M)^{-1}\| = \|(H_V + \rho_M)^{-1}(\rho_M - \Delta)\| \le \frac{1}{C_M}. \tag{3.7}$$

Proof. We decompose by means of (3.5)

$$(H_V + \rho_M)^{-1}(\rho_M - \Delta) = R_V R_0^{-1} = 1 + V R_V$$

and estimate the operator norm:

$$\|(H_V + \rho_M)^{-1}(\rho_M - \Delta)\| \le 1 + \|V\|_{L^2} \|R_V\|_{\mathcal{B}(L^2, L^\infty)}. \tag{3.8}$$

Now we get the assertion by the following lemma. □

Lemma 3.3. *The resolvents* (3.6) *of the Schrödinger operators* (2.3) *are uniformly bounded in $\mathcal{B}(L^2, L^\infty)$ for all potentials $V \in \mathcal{M}$.*

Proof. The set $\{R_V : V \in \mathcal{M}\}$ is bounded in $\mathcal{B}(L^2, L^\infty)$ iff

$$\{\phi : (\Delta - \rho_M - V)\phi = \psi, \ \|\psi\|_{L^2} \le 1, \ V \in \mathcal{M}\} \tag{3.9}$$

is bounded in $L^\infty(\Omega)$.
According to Theorem 2.1 the distance of $-\rho_M$ to the spectrum of the operator $-\Delta + V$ is at least 1 and thus $\|(\Delta - \rho_M - V)^{-1}\|_{\mathcal{B}(L^2, L^2)} \le 1$. Hence the set (3.9) lies within the unit ball of $L^2(\Omega)$. This implies

$$\|\psi + V\phi\|_{L^1} \le \sqrt{|\Omega|} + M, \quad \forall V \in \mathcal{M}, \ \|\psi\|_{L^2} \le 1$$

for all ϕ from (3.9), i.e. the set

$$\{\psi + V\phi : (\Delta - \rho_M)\phi = \psi + V\phi, \ \|\psi\|_{L^2} \le 1, \ V \in \mathcal{M}\} \tag{3.10}$$

is bounded in $L^1(\Omega)$. The embedding $L^1(\Omega) \hookrightarrow W^{-1,p}$ is continuous for $1 \leq p < \frac{d}{d-1}$, hence for these p the set (3.10) is bounded in $W^{-1,p}(\Omega)$. As $\Delta - \rho_M$ is a continuous bijection from $W_0^{1,p}(\Omega)$ onto $W^{-1,p}(\Omega)$ for $p_0/(p_0-1) \leq p \leq p_0$ (cf. (1.13)), now follows that the set (3.9) is H_0^1–bounded in the one–dimensional case ($d=1$) and in general $W_0^{1,p}$–bounded if $\frac{p_0}{p_0-1} \leq p < \frac{d}{d-1}$. This implies the L^q–boundedness of (3.9) for

- $q = \infty$ in the one–dimensional case ($d=1$),
- $1 \leq q < \infty$ in the two–dimensional case ($d=2$),
- $1 \leq q \leq 3$ in the three–dimensional case ($d=3$),

according to Sobolev's Embedding Theorem. As

$$\|\psi + V\phi\|_{L^r} \leq |\Omega|^{1/r}\|\psi\|_{L^2} + \|V\|_{L^2}\|\phi\|_{L^q} \quad 1/r = 1/2 + 1/q$$

now follows the L^r–boundedness of the set (3.10) for

- $1 \leq r < 2$ in the two–dimensional case ($d=2$),
- $1 \leq r \leq 3/2$ in the three–dimensional case ($d=3$).

By embedding (3.10) is bounded in $W^{-1,p}(\Omega)$ for

- $1 \leq p < \infty$ in the two–dimensional case ($d=2$),
- $1 \leq p \leq 3$ in the three–dimensional case ($d=3$).

If $p_0/(p_0-1) \leq p \leq \min\{3, p_0\}$ the bijection $(\Delta - \rho_M)^{-1} \in \mathcal{B}\left(W^{-1,p}, W_0^{1,p}\right)$ maps the $W^{-1,p}(\Omega)$–bounded set (3.10) onto (3.9) which thus turns out to be a bounded set in $W_0^{1,p}(\Omega)$.
In the **two–dimensional case** ($d=2$) now immediately follows the L^∞–boundedness of the set (3.9) because $W_0^{1,p}(\Omega)$ is continuously embedded into $L^\infty(\Omega)$ for all $p > 2$.
In the **three–dimensional case** ($d=3$) we have to reiterate our argument once again. From the $W_0^{1,3}$–boundedness of (3.9) one obtains by embedding the L^q–boundedness for $1 \leq q < \infty$. Hence the set (3.10) is L^r–bounded for $1 \leq r < 2$ and via embedding it is $W^{-1,p}$–bounded for $1 \leq p < 6$. Application of $(\Delta - \rho_M)^{-1} \in \mathcal{B}\left(W^{-1,p}, W_0^{1,p}\right)$ now provides the $W_0^{1,p}$–boundedness of the set (3.9) for some $p > 3$ and thus by embedding its L^∞–boundedness. $\square$

Corollary 3.3. *Let be $\mathcal{M}_1$ and $\mathcal{M}_2$ two bounded sets in $L^2(\Omega)$. The set*

$$\{WR_V \, : \, W \in \mathcal{M}_1, V \in \mathcal{M}_2\} \tag{3.11}$$

is bounded in $\mathcal{B}(L^2)$ by

$$\sup_{W \in \mathcal{M}_1} \|W\|_{L^2} \sup_{V \in \mathcal{M}_2} \|R_V\|_{\mathcal{B}(L^2, L^\infty)}.$$

Corollary 3.4. *The eigenfunctions $\{\psi_l(V)\}_{l=1}^\infty$ of the Schrödinger operator* (2.3) *are continuous on $\overline{\Omega}$ and there is*

$$\|\psi_l(V)\|_{C(\overline{\Omega})} \leq \frac{c}{C_M}\left(\epsilon_l(V) + \rho_M\right), \quad l = 1, 2, \dots, \quad \forall V \in \mathcal{M}, \tag{3.12}$$

$\epsilon_l(V)$ being the eigenvalue of the Schrödinger operator H_V corresponding to $\psi_l(V)$.

Proof. The eigenfunctions $\psi_l = \psi_l(V)$ belong to $H^2(\Omega)$ which is continuously embedded into $C(\overline{\Omega})$. There is for all $V \in \mathcal{M}$ (recall Theorem 3.1 and (2.2))

$$\begin{aligned} \|\psi_l\|_{C(\overline{\Omega})} &\leq c_0 \|\psi_l\|_{H^2} \leq c\,\|(\rho_M - \Delta)\psi_l\|_{L^2} \leq \frac{c}{C_M}\|(H_V + \rho_M)\psi_l\|_{L^2} \\ &= \frac{c}{C_M}\|(\epsilon_l + \rho_M)\psi_l\|_{L^2} = \frac{c}{C_M}(\epsilon_l + \rho_M) \quad l = 1, 2, \dots , \end{aligned}$$

where $\epsilon_l = \epsilon_l(V)$. □

3.5. Dependence on the complex argument. Let $H = \int_{-\infty}^{\infty} \lambda dE(\lambda)$ be the spectral decomposition of the (self–adjoint) Schrödinger operator (2.3). For all $z \in \mathcal{C}$, $z \notin \sigma(H)$ there is

$$\begin{aligned} &\|(z - H)^{-1}(H + \rho_M)\| = \|(H + \rho_M)(z - H)^{-1}\| \\ &= \left| \int_{-\infty}^{\infty} \frac{\lambda + \rho_M}{z - \lambda} d\|E(\lambda)\| \right| \leq \left(\sup_{\lambda \in \sigma(H)} \left| \frac{\lambda + \rho_M}{z - \lambda} \right| \right) \int_{-\infty}^{\infty} d\|E(\lambda)\| \\ &\leq \sup_{\lambda \in \sigma(H)} \left(1 + \frac{|z + \rho_M|}{|z - \lambda|} \right) \leq 1 + \frac{\rho_M + |z|}{\operatorname{dist}(z, \sigma(H))}. \end{aligned}$$

(N.B. the operators $(H + \rho_M)$ and $(z - H)^{-1}$ commute, as self–adjoint operators commute with their resolvents.) There follows for all $V \in L^2(\Omega)$, $\|V\|_{L^2} \leq M$ and $z \in \mathcal{C}$, $\operatorname{dist}(z, [\sigma_M, \infty)) \geq \delta$

$$\|(z - H)^{-1}(H + \rho_M)\| = \|(H + \rho_M)(z - H)^{-1}\| \leq 1 + \frac{\rho_M + |z|}{\delta}\,. \tag{3.13}$$

Lemma 3.4. *For all potentials $V \in L^2(\Omega)$ with $\|V\|_{L^2} \leq M$ and all $z \in \mathcal{C}$ with* $\operatorname{dist}(z, [\sigma_M, \infty)) \geq \delta$ *there is for the resolvent $(z - H_V)^{-1}$ of the Schrödinger operator* (2.3)

$$\|(\rho_M - \Delta)(z - H_V)^{-1}\| = \|(z - H_V)^{-1}(\rho_M - \Delta)\| \leq C_{M\delta}(1 + |z|) \tag{3.14}$$

where $C_{M\delta} = \frac{\rho_M + \delta}{C_{M\delta}}$, $\rho_M = 1 - \sigma_M$ and σ_M as defined in (2.4).

Proof. We decompose

$$\begin{aligned} (\rho_M - \Delta)(z - H_V)^{-1} &= (\rho_M - \Delta)(H_V + \rho_M)^{-1}(H_V + \rho_M)(z - H_V)^{-1} \\ (z - H_V)^{-1}(\rho_M - \Delta) &= (z - H_V)^{-1}(H_V + \rho_M)(H_V + \rho_M)^{-1}(\rho_M - \Delta) \end{aligned}$$

and estimate by means of (3.13) and Theorem 3.1. □

Using this result we can state for the resolvents of the Schrödinger operators corresponding to potentials from the M–ball in $L^2(\Omega)$ estimates which are analogous to those for the resolvent of the Laplacian from Sections 3.1 and 3.2. From the Lemmata 3.1, 3.4 and Corollary 3.1 follows immediately

Proposition 3.1. *Let be V a potential from the M–ball in $L^2(\Omega)$ and z a complex number with* $\operatorname{dist}(z, [\sigma_M, \infty)) \geq \delta$*. Then the resolvent $(z - H_V)^{-1}$ of the Schrödinger operator* (2.3) *belongs to the summability–class $\mathcal{B}_p$ for all $p > d/2$. Moreover there is for all $\alpha > 0$*

$$(z - H_V)^{-\alpha} \in \mathcal{B}_p, \quad \forall p > d/(2\alpha). \tag{3.15}$$

Proposition 3.2. *Let be $U, V \in L^2(\Omega)$, $M = \|V\|_{L^2}$, z a complex number with* $\operatorname{dist}(z, [\sigma_M, \infty)) \geq \delta$ *and* $H_V = -\Delta + V$ *the Schrödinger operator* (2.3). *Then* $U(z - H_V)^{-1} \in \mathcal{B}_p$, *for all* $p > 2d$ *and*

$$\|U(z - H_V)^{-1}\|_p \leq c\, C_{M\delta}(1 + |z|)\|U\|_{L^2}. \tag{3.16}$$

Proof. We decompose

$$U(z - H_V)^{-1} = -U(\Delta - \rho_M)^{-1}(\Delta - \rho_M)(z - H_V)^{-1}$$

and estimate by means of Hölder's inequality

$$\|U(z - H_V)^{-1}\|_p \leq \|U(\Delta - \rho_M)^{-1}\|_p \|(\Delta - \rho_M)(z - H_V)^{-1}\|.$$

Now the assertion follows from the Lemmata 3.2 and 3.4. □

By means of Propositions 3.1, 3.2 one obtains

$$(z - H_{V_1})^{-1}U(z - H_{V_2})^{-1} \in \mathcal{B}_p,$$

$$\left\|(z - H_{V_1})^{-1}U(z - H_{V_2})^{-1}\right\|_p \leq c\, C_{M\delta}^2(1 + |z|)^2\|U\|_{L^2},\ M = \max\{\|V_1\|_{L^2}, \|V_2\|_{L^2}\},$$

$$\forall p > 2d/5, \quad \forall U, V_1, V_2 \in L^2(\Omega), \quad \forall z \in \mathbf{C},\ \operatorname{dist}(z, [\sigma_M, \infty)) \geq \delta.$$

Thus, in the two-dimensional case ($d = 2$) the operators $(z - H_{V_1})^{-1}U(z - H_{V_2})^{-1}$ are nuclear. In the three-dimensional case ($d = 3$) any product of two resolvents $(z - H_{V_j})^{-1}$, $j = 1, 2$ and one operator $U(z - H_V)^{-1}$ is nuclear; more precisely

Proposition 3.3. *Let be $U, V, V_1, V_2 \in L^2(\Omega)$, $M = \max\{\|V\|_{L^2}, \|V_1\|_{L^2}, \|V_2\|_{L^2}\}$, z a complex number with* $\operatorname{dist}(z, [\sigma_M, \infty)) \geq \delta$ *and H_V, H_{V_1}, H_{V_2} the Schrödinger operators* (2.3) *with potentials V, V_1, V_2, respectively. Then all first order products of the operators $(z - H_{V_1})^{-1}$, $(z - H_{V_2})^{-1}$ and $U(z - H_V)^{-1}$ belong to the summability-class $\mathcal{B}_p$ for all $p > 2d/9$ and have equal $\mathcal{B}_p$-norm. There is*

$$\left\|(z - H_{V_1})^{-1}U(z - H_V)^{-1}(z - H_{V_2})^{-1}\right\|_p \leq c\, C_{M\delta}^3(1 + |z|)^3\|U\|_{L^2}.$$

4. Functions of the Schrödinger operator

Ultimately we are interested in the Fréchet derivative of $\operatorname{tr}(\mathfrak{f}(H_V))$ with respect to the potential V, where H_V is the Schrödinger operator (2.3) and $\mathfrak{f}$ is the positive decreasing distribution function f or one of its primitive functions. We have got p-summability of the resolvent of the Schrödinger operator H_V. Now we are looking for a suitable representation of $\mathfrak{f}(H_V)$ in terms of the resolvent of H_V. Nier based his calculations on the following one due to Helffer and Sjöstrand [7]:
Let be H a self-adjoint operator in a Hilbert space, $\mathfrak{f} \in C_0^\infty(\mathbf{R})$ and $\mathfrak{F} \in C_0^\infty(\mathbf{C})$ an extension of $\mathfrak{f}$ such that $\partial_{\bar{z}}\mathfrak{F} = 0$ on the real axis. Then there is

$$\mathfrak{f}(H) = \frac{i}{2\pi}\int_{\mathbf{C}} \partial_{\bar{z}}\mathfrak{F}(z)(z - H)^{-1} d\bar{z} \wedge dz\ .$$

In the present context, however, this construction is rather complicated, because the distribution function has not finite support. One may raise the question whether a Dunford integral of the form

$$\mathfrak{f}(H_V) = \frac{1}{2\pi i}\int_\Gamma \mathfrak{f}(z)(z - H_V)^{-1} dz$$

cannot be used, where Γ is an orientated contour 'enclosing' the spectrum of H_V. This seems possible as the spectrum of H_V is uniformly bounded from below for all potentials from a ball in L^2 and indeed it can be done.

4.1. Functional calculus. For any $\rho \in \mathbf{R}$ and $\delta > 0$ we define

$$K = K_{\rho,\delta} = \{z \in \mathbf{C} : \operatorname{dist}([\rho, \infty), z) \leq \delta\}. \tag{4.1}$$

A path Γ is said to be admissible with respect to $K = K_{\rho,\delta}$, or K–admissible, if $\Gamma \subset K$ is a piecewise continuously differentiable orientated contour with $\Gamma \cap [\rho, \infty) = \emptyset$, surrounding the half–axis $[\rho, \infty)$ in such a way that it always lies on the left–hand side. Let be $G \supset K$ a region in $\mathbf{C}$ and let us assume throughout this section

$$\mathfrak{f} \in \mathcal{O}(G), \quad \int_{\partial K} |\mathfrak{f}(z)| dz < \infty, \quad \|\mathfrak{f}\|_{L^\infty(K)} < \infty, \tag{4.2}$$

where $\mathcal{O}(G)$ denotes the $\mathbf{C}$–algebra of all holomorphic functions in the domain G [13].

Lemma 4.1. *For any $K_{\rho,\delta}$–admissible contour Γ there is*

$$\mathfrak{f}(\lambda) = \frac{1}{2\pi i} \int_\Gamma \frac{\mathfrak{f}(z)}{z - \lambda}\, dz, \quad \forall \lambda \in [\rho, \infty). \tag{4.3}$$

Proof. Let be $j > \rho$ arbitrary and

$$\begin{array}{rclrcl} \{z_j^+\} &=& \{z \in \Gamma : \Re z = j,\ \Im z > 0\} & \{z_j^-\} &=& \{z \in \Gamma : \Re z = j,\ \Im z < 0\} \\ \Gamma_j &=& \{z \in \Gamma : \Re z < j\} & \gamma_j &=& \{z \in \partial K : \Re z < j\}, \\ \tilde{\Gamma}_j &=& [z_j^-, z_j^+] & \tilde{\gamma}_j &=& [j - i\delta, z_j^-] \cup [j + i\delta, z_j^+]. \end{array}$$

Now let be $\lambda \in [\rho, \infty)$ and j any integer with $j > \lambda + 1$. According to Cauchy's Curvilinear Integral Theorem we have

$$\mathfrak{f}(\lambda) = \frac{1}{2\pi i} \int_{\Gamma_j \cup \tilde{\Gamma}_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz = \frac{1}{2\pi i} \int_{\Gamma_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz + \frac{1}{2\pi i} \int_{\tilde{\Gamma}_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz.$$

The first integral on the right–hand side is uniformly bounded for all $\lambda \in [\rho, \infty)$ and $j > \lambda + 1$:

$$\left| \int_{\Gamma_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz \right| \leq \left| \int_{\gamma_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz \right| + \left| \int_{\tilde{\gamma}_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz \right| \leq \frac{1}{\delta} \int_{\gamma_j} |\mathfrak{f}(z)|\ dz + 2\delta \|\mathfrak{f}\|_{L^\infty(K)}.$$

In the limit $j \to \infty$ we have by Lebesgue's Dominated Convergence Theorem

$$\lim_{j \to \infty} \int_{\Gamma_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz = \int_\Gamma \frac{\mathfrak{f}(z)}{z - \lambda} dz.$$

The remaining integral tends to zero as $j \to \infty$ because of

$$\left| \int_{\tilde{\Gamma}_j} \frac{\mathfrak{f}(z)}{z - \lambda} dz \right| \leq \frac{2\delta}{j - \lambda} \|\mathfrak{f}\|_{L^\infty(K)}.$$

□

Corollary 4.1. *Under the assumptions of Lemma* 4.1 *there is*

$$\mathfrak{f}^{(k)}(\lambda) = \frac{k!}{2\pi i}\int_\Gamma \frac{\mathfrak{f}(z)}{(z-\lambda)^{k+1}}\,dz, \quad k=0,1,\dots, \quad \forall\lambda\in[\rho,\infty). \tag{4.4}$$

Theorem 4.1. *Let be H a self-adjoint semi-bounded operator in a Hilbert space and ρ any real number which is not greater than the lower bound of H. Then the Dunford integral over any $K_{\rho,\delta}$-admissible contour Γ with positive distance to the half-axis $[\rho,\infty)$ equals $\mathfrak{f}(H)$*

$$\mathfrak{f}(H) = \frac{1}{2\pi i}\int_\Gamma \mathfrak{f}(z)(z-H)^{-1}\,dz. \tag{4.5}$$

Proof. Let's regard the spectral decomposition $H=\int_{-\infty}^{\infty}\lambda dE(\lambda)$ of H. Then

$$(z-H)^{-1} = \int_{-\infty}^{\infty}\frac{1}{z-\lambda}dE(\lambda), \quad \mathfrak{f}(H)=\int_{-\infty}^{\infty}\mathfrak{f}(\lambda)dE(\lambda).$$

By means of Lemma 4.1 and Fubini's Theorem we can justify the following calculations

$$\begin{aligned}\mathfrak{f}(H) &= \int_{-\infty}^{\infty}\mathfrak{f}(\lambda)dE(\lambda) = \int_{-\infty}^{\infty}\frac{1}{2\pi i}\int_\Gamma\frac{\mathfrak{f}(z)}{z-\lambda}\,dz\,dE(\lambda)\\ &= \frac{1}{2\pi i}\int_\Gamma \mathfrak{f}(z)\int_{-\infty}^{\infty}\frac{dE(\lambda)}{z-\lambda}\,dz = \frac{1}{2\pi i}\int_\Gamma \mathfrak{f}(z)(z-H)^{-1}\,dz.\end{aligned}$$

N.B. $\mathfrak{f}dz\otimes dE(\lambda)$ is a bounded measure on $\Gamma\times[\rho,\infty)$ and $|\frac{1}{z-\lambda}|\le\frac{1}{\mathrm{dist}([\rho,\infty),\Gamma)}$ for $z\in\Gamma$, $\lambda\in[\rho,\infty)$. □

Corollary 4.2. *Under the assumptions of Theorem* 4.1 *there is*

$$\mathfrak{f}^{(k)}(H) = \frac{k!}{2\pi i}\int_\Gamma \mathfrak{f}(z)(z-H)^{-(k+1)}\,dz, \quad k=0,1,\dots. \tag{4.6}$$

Observing Theorem 2.1 we now get

Corollary 4.3. *Let be $M>0$, H_V the Schrödinger operator* (2.3) *corresponding to a potential $V\in L^2(\Omega)$ with $\|V\|_{L^2}\le M$, σ_M as defined in* (2.4), *$y\in\mathbf{R}$ arbitrary and $\rho<\sigma_M-y$. Then for any $K_{\rho,\delta}$-admissible contour Γ with positive distance to the half-axis $[\rho,\infty)$ there is*

$$\mathfrak{f}^{(k)}(H_V-y) = \frac{k!}{2\pi i}\int_\Gamma \mathfrak{f}(z)(z-H_V+y)^{-(k+1)}\,dz, \quad k=0,1,\dots. \tag{4.7}$$

Remark 4.1. We can choose in particular $\Gamma=\partial K$, $K=K_{\rho,\delta}$ according to (4.1), as a K-admissible path with positive distance to the half axis $[\rho,\infty)$ which we will frequently do in the following applications.

4.2. The distribution function f and its primitive functions. In §1 we asked the distribution function f to be positive, strictly decreasing and vanishing towards $+\infty$ in such a way that $F(s) = -\int_s^\infty f(t)dt$ exists. Provided all the integrals involved are finite we denote by

$$f^{(-j)}(s) := -\int_s^\infty f^{(1-j)}(t)dt, \quad j = 1, 2, \dots, \quad f^{(0)} := f \tag{4.8}$$

the iterated primitive functions of f which tend to zero while the argument approaches $+\infty$. The functions $(-1)^j f^{(-j)}$ are positive and strictly decreasing and if $f^{(-j)}$exists there is $\lim_{t\to\infty} t|f^{(1-j)}(t)| = 0$.
In view of the functional calculus from §4.1 we will assume that f is the trace of some holomorphic function in a region G covering the real line. More precisely G shall be a region in $\mathbf{C}$ which is symmetric about $\mathbf{R}$ with the following property

$$\forall \rho \in \mathbf{R}\, \exists \delta > 0 \quad K_{\rho,\delta} \subset G. \tag{4.9}$$

With regard to the distribution function f we assume

$$f \in \mathcal{O}(G), \quad f(G \cap \mathbf{R}) \subset (0, +\infty), \quad f'(G \cap \mathbf{R}) \subset (-\infty, 0). \tag{4.10}$$

The reality of f on $\mathbf{R}$ can equivalently be expressed as $f(\bar{z}) = \bar{f}(z)$ for all $z \in G$.
N.B. f has primitive functions which are holomorphic in G and real–valued on $\mathbf{R}$.
Further we have to impose a decay property on the primitives of f:

$$\int_\rho^\infty \left|f^{-k}(t+i\delta)\right| |t|^\nu dt < \infty, \quad \forall \rho \in \mathbf{R}, \quad (k,\nu) = (1,4), (2,4), (3,6), \tag{4.11}$$

where $\delta = \delta(\rho)$ is as in (4.9). (4.11) ensures together with the holomorphy of f in G and the reality of f on $\mathbf{R}$ the existence of the integrals

$$\int_{\partial K_{\rho,\delta}} \left|f^{-k}(z)\right| (1 + |z|^\nu)\, dz < \infty, \quad \forall \rho \in \mathbf{R}, \tag{4.12}$$
$$(k,\nu) \in (1,[0,4]) \cup (2,[0,4]) \cup (3,[0,6]),$$

for the sets $K = K_{\rho,\delta}$ from (4.9). We need the property (4.12) with $(k,\nu) = (3,6)$ in order to prove the uniform boundedness of the electron density (cf. Proposition 6.1) and we require it with $(k,\nu) = (1,4)$ and $(k,\nu) = (2,4)$ to get the Fréchet–differentiability (with respect to the potential V) of the operator $f(H_V - \epsilon_0(V))$ and $F(H_V - \epsilon_0(V))$ respectively (cf. Lemma 6.1).

Remark 4.2. The class (4.10), (4.11) covers all the physically relevant distribution functions, such as the decaying exponential $e^{-\alpha t}$, $\alpha > 0$ and $\frac{\beta}{1+e^{\alpha t}}$, $\alpha, \beta > 0$.
By means of the functional calculus we can prove

Theorem 4.2. *Let be H the Schrödinger operator* (2.3) *with an arbitrary potential $V \in L^2(\Omega)$. Then $f(H)$ and $F(H)$ are nuclear operators in $L^2(\Omega)$, where f is a distribution function with* (4.10),(4.11) *and $F = f^{(-1)}$ the corresponding primitive* (4.8).

Proof. Let be $j = 0$ or $j = 1$. According to Corollary 4.3 there is

$$f^{(-j)}(H) = \frac{2!}{2\pi i} \int_{\partial K} f^{(-j-2)}(z)(z-H)^{-3}\, dz\,,$$

where $K = K_{\sigma_M,\delta(\sigma_M)}$, $M = \|V\|_{L^2}$. We know that $(z-H)^{-3}$ is nuclear (cf. Proposition 3.3, take $U \equiv 1$), thus

$$\|f^{(-j)}(H)\|_1 \le \frac{1}{\pi}\int_{\partial K} |f^{(-j-2)}(z)|\; \|(z-H)^{-3}\|_1\, dz$$
$$\le \frac{c}{\pi} C^3_{M\delta} \int_{\partial K} |f^{(-j-2)}(z)|(1+|z|)^3 dz \;<\; \infty.$$

The right–hand side of this inequality is finite according to (4.12). □

4.3. Differentiation with respect to potentials from $L^2(\Omega)$. We will now establish the Fréchet–differentiability of the function

$$\mathcal{F}_0 \in \left(L^2(\Omega) \to \mathcal{B}_1\right), \quad \mathcal{F}_0(V) := F(H_V) \tag{4.13}$$

which depends on the potential V of the Schrödinger operator (2.3) and where F is the primitive function (4.8) of the distribution function f. The procedure is analogous to that in [11], though by admitting potentials from $L^2(\Omega)$ one has to regard higher order resolvent terms.

Theorem 4.3. *The function* (4.13) *is Fréchet differentiable for every* $V \in L^2(\Omega)$ *and the derivative* $\mathcal{F}_0'(V) \in \mathcal{B}(L^2(\Omega), \mathcal{B}_1)$ *is given by*

$$\mathcal{F}_0'(V)[W] = \frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\left(R^2WR + RWR^2\right)\, dz, \quad \forall W \in L^2(\Omega), \tag{4.14}$$

where $R = R(z) = (z-H)^{-1}$ *is the resolvent of the Schrödinger operator* (2.3) *and* Γ *is any* K*–admissible contour with positive distance to the half–axis* $[\sigma_M, \infty)$. σ_M *is as in* (2.5) *with* $M > \|V\|_{L^2}$ *and* $K = K_{\sigma_M,\delta(\sigma_M)}$ *is the set* (4.1) *with the* δ *from* (4.9).

Proof. Indeed, $\mathcal{F}_0'(V) \in \mathcal{B}(L^2(\Omega), \mathcal{B}_1)$, because by Proposition 3.3 (also recall Remark 4.1, (4.9) and (4.1)) there is for any $W \in L^2(\Omega)$

$$\begin{aligned} \|\mathcal{F}_0'(V)[W]\|_1 &\le \frac{1}{2\pi}\int_{\partial K} |f^{(-2)}(z)|\,\left\|R^2WR + RWR^2\right\|_1 dz \\ &\le \frac{c}{2\pi} C^3_{M\delta}\|W\|_{L^2}\int_{\partial K} |f^{(-2)}(z)|\,(1+|z|)^3\, dz \end{aligned}$$

and the integral on the right–hand side is finite according to (4.12). Without loss of generality let be $W \in L^2(\Omega)$ such that $\|V+W\|_{L^2} \le M$. Then

$$\mathcal{F}_0(V+W) - \mathcal{F}_0(V) = \frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\left((z-(H+W))^{-2} - (z-H)^{-2}\right)\, dz\, .$$

Now we decompose the difference of the resolvent–squares (cf. §3.3) under the integral

$$R_W^2 - R^2 = R^2WR + RWR^2 + RR_W(WR)^2 + R_W(WR)^2R + (R_WWR)^2$$

where $R = R(z) = (z-H)^{-1}$ and $R_W = R_W(z) = (z-(H+W))^{-1}$. The first two terms are the contribution to the derivative and we get for the remainder of the linear expansion of $\mathcal{F}_0(V+W)$ at V

$$\begin{aligned}\omega(V,W) &= \mathcal{F}_0(V+W) - \mathcal{F}_0(V) - \mathcal{F}_0'(V)[W] \\ &= \frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\ \left(RR_W(WR)^2 + R_W(WR)^2R + (R_WWR)^2\right)\ dz.\end{aligned}$$

By means of Proposition 3.2, Proposition 3.3 and (4.12) we can estimate the nuclear norm of the remainder

$$\|\omega(V,W)\|_1 \le \frac{c}{2\pi} C_{M6}^4 \|W\|_{L^2}^2 \int_{\partial K} |f^{(-2)}(z)|\,(1+|z|)^4\,dz \ < \ \infty.$$

Thus we have received the desired result

$$\frac{\|\omega(V,W)\|_1}{\|W\|_{L^2}} \to 0 \quad \text{as} \quad \|W\|_{L^2} \to 0\,.$$

□

Remark 4.3. One gets higher derivatives of $\mathcal{F}_0(V)$ by further decomposing the difference of the resolvent–squares $R_W^2 - R^2$. Thus one obtains for the second order term in the Taylor expansion

$$\mathcal{F}_0(V+W) = \mathcal{F}_0(V) + \mathcal{F}_0'(V)[W] + \frac{1}{2}\mathcal{F}_0''(V)[W,W] + \dots$$

$$\mathcal{F}_0''(V)[W,W] = \frac{2!}{2\pi i}\int_\Gamma f^{(-2)}(z)\left(R^2(WR)^2 + R(WR)^2R + (RWR)^2\right)dz, \tag{4.15}$$

where $R = (z-H_V)^{-1}$. The nuclear norm of the corresponding remainder is a $o(\|W\|_{L^2}^2)$.

If the operators W and $R = (z-H)^{-1}$ commuted, there would be

$$\begin{aligned}\mathcal{F}_0'(V)[W] &= \frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\left(R^2WR + RWR^2\right)\ dz \\ &= \left(\frac{2}{2\pi i}\int_\Gamma f^{(-2)}(z)(z-H)^{-3}\,dz\right)\ W \ = \ f(H)\,W,\end{aligned}$$

i. e. $\mathcal{F}_0'(V) = f(H)$. In general, however, the operators W and $(z-H)^{-1}$ do not commute, but we get something of the above under the trace, as $\mathrm{tr}(AB) = \mathrm{tr}(BA)$.

Theorem 4.4. *The functional*

$$\phi_0 \in \left(L^2(\Omega) \to \mathbf{R}\right), \quad \phi_0(V) = \mathrm{tr}(\mathcal{F}_0(V)) = \mathrm{tr}(F(H_V)) \tag{4.16}$$

is Fréchet differentiable for every $V \in L^2(\Omega)$ and the derivative $\phi_0'(V) \in (L^2(\Omega))^* \equiv L^2(\Omega)$ is given by

$$\langle \phi_0'(V), W\rangle = \mathrm{tr}\,(f(H_V)\,W)\,, \quad \forall W \in L^2(\Omega). \tag{4.17}$$

Proof. Let be $V \in L^2(\Omega)$ arbitrary and fixed, $M > \|V\|_{L^2}$ and without loss of generality $W \in L^2(\Omega)$ such that $\|V+W\|_{L^2} \le M$. Each term in the linear expansion

$$\mathcal{F}_0(V+W) = \mathcal{F}_0(V) + \mathcal{F}_0'(V)[W] + \omega(V,W)$$

of $\mathcal{F}_0(V+W)$ is nuclear and by applying the continuous linear functional tr we get

$$\phi_0(V+W) = \phi_0(V) + \mathrm{tr}(\mathcal{F}_0'(V)[W]) + \mathrm{tr}(\omega(V,W)).$$

Let us first estimate the remainder

$$|\operatorname{tr}(\omega(V,W))| \le \|\omega(V,W)\|_1 = o(\|W\|_{L^2}).$$

$\operatorname{tr}(\mathcal{F}_0'(V)[W])$ is indeed the Fréchet derivative $\phi_0'(V)$ applied to W, because the composition $\operatorname{tr}\circ\mathcal{F}_0'(V):\ L^2(\Omega) \xrightarrow{\mathcal{F}_0'(V)} \mathcal{B}_1 \xrightarrow{\operatorname{tr}} \mathbf{R}$ is a continuous linear functional. Now we calculate the derivative explicitly, using the relation $\operatorname{tr}(AB) = \operatorname{tr}(BA)$

$$\begin{aligned}\langle \phi_0'(V), W\rangle &= \operatorname{tr}(\mathcal{F}_0'(V)[W]) = \frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\operatorname{tr}\left(R^2WR + RWR^2\right)\,dz \\ &= \frac{2}{2\pi i}\int_\Gamma f^{(-2)}(z)\operatorname{tr}\left((z-H_V)^{-3}\,W\right)\,dz \\ &= tr\left(\frac{2}{2\pi i}\int_\Gamma f^{(-2)}(z)(z-H_V)^{-3}\,dz\,W\right) = tr\left(f(H_V)\,W\right)\end{aligned}$$

where Γ is as in Theorem 4.3. □

5. The Fermi level $\epsilon_0(V)$

The Fermi level ϵ_0 as a function of the potential V is implicitly defined by the electric–neutrality equation

$$\bar{n}_D = \int_\Omega n_D(x)dx = \int_\Omega n(x)dx = \sum_{l=1}^{\infty} f(\epsilon_l(V) - \epsilon_0(V)), \tag{5.1}$$

where $\{\epsilon_l(V)\}_{l=1}^{\infty}$ are the eigenvalues in increasing order (counting multiplicity) of the Schrödinger operator (2.3) with the potential $V \in L^2(\Omega)$. Indeed, for every $V \in L^2(\Omega)$ the Fermi level $\epsilon_0(V)$ is uniquely determined that way, as the series

$$g(V,y) = \sum_{l=1}^{\infty} f(\epsilon_l(V) - y) = \operatorname{tr}(H_V - y),\quad V \in L^2(\Omega),\ y \in \mathbf{R} \tag{5.2}$$

converges according to Theorem 4.2 and defines a positive and (strictly) increasing function $g_V(y) = g(V,y)$ with the property

$$\lim_{y\to\infty} g_V(y) = \infty,\quad \lim_{y\to-\infty} g_V(y) = 0.$$

The function $g \in (L^2(\Omega)\times\mathbf{R} \to \mathbf{R})$ has continuous partial derivatives

$$\partial_1 g(V,y) \in \mathcal{B}(L^2(\Omega),\mathbf{R}) \equiv L^2(\Omega),\qquad \partial_2 g(V,y) \in \mathcal{B}(\mathbf{R},\mathbf{R}) \equiv \mathbf{R}$$

on $L^2(\Omega)\times\mathbf{R}$

$$\langle \partial_1 g(V,y), W\rangle \;=\; \operatorname{tr}(f'(H_V - y)W),\quad \forall W \in L^2(\Omega) \tag{5.3}$$

$$\partial_2 g(V,y) \;=\; -\operatorname{tr}(f'(H_V - y)) \;=\; -\sum_{l=1}^{\infty} f'(\epsilon_l(V) - y) > 0. \tag{5.4}$$

Thus, by the Implicit Function Theorem for every $\tilde{V} \in L^2(\Omega)$ there is a neighborhood $\tilde{\mathcal{M}} \subset L^2(\Omega)$ of $\tilde{V}$ and a continuously Fréchet–differentiable function $\epsilon_0 \in \left(\tilde{\mathcal{M}} \to \mathbf{R}\right)$ such that

$$g(V,\epsilon_0(V)) = \bar{n}_D,\quad \forall V \in \tilde{\mathcal{M}}$$

and the Fréchet–derivative $\epsilon_0' \in \left(\tilde{\mathcal{M}} \to L^2(\Omega)\right)$ is given by

$$\langle \epsilon_0'(V), W \rangle = \frac{\mathrm{tr}(f'(H_V - \epsilon_0(V))W)}{\mathrm{tr}(f'(H_V - \epsilon_0(V)))}, \quad \forall W \in L^2(\Omega),\ \forall V \in \tilde{\mathcal{M}}. \tag{5.5}$$

This implies that $\epsilon_0 \in (L^2(\Omega) \to \mathbf{R})$ is a continuously Fréchet–differentiable function on every compact subset of $L^2(\Omega)$. NIER [11] used the M–ball of $H^1(\Omega)$ as such a set. We want to extend the result to the M–ball of $L^2(\Omega)$.

Theorem 5.1. *Let be $M > 0$ arbitrary and $\mathcal{M}$ the closed M-ball in $L^2(\Omega)$. Then the mapping $\epsilon_0 \in ((\mathcal{M}, \mathrm{wk}) \to \mathbf{R})$ is continuous.*

Proof. Assume the mapping $\epsilon_0 \in ((\mathcal{M}, \mathrm{wk}) \to \mathbf{R})$ were not continuous. Then there is a sequence $\{V_l\}_{l=1}^{\infty} \subset \mathcal{M}$ and a $V \in \mathcal{M}$ with $V_l \rightharpoonup V$ weakly in $L^2(\Omega)$ such that

$$|\epsilon_0(V_l) - \epsilon_0(V)| > \delta_0 > 0, \quad \forall l = 1, 2, \dots \,. \tag{5.6}$$

Let be $H = H_V = -\Delta + V$ and $H_l = H_{V_l} = -\Delta + V_l$ the Schrödinger operators (2.3) corresponding to the potentials V and V_l, $l = 1, 2, \dots$, respectively. We abbreviate $\epsilon_0 := \epsilon_0(V)$ and $\epsilon_{0l} := \epsilon_0(V_l)$, $l = 1, 2, \dots$. According to the electric–neutrality condition (5.1) we have

$$\bar{n}_D = \mathrm{tr}\,(f(H_l - \epsilon_{0l})) = \mathrm{tr}\,(f(H - \epsilon_0)), \quad \forall l = 1, 2, \dots\,,$$

i.e. for all $l = 1, 2, \dots$ there is

$$\mathrm{tr}\,(f(H_l - \epsilon_{0l}) - f(H_l - \epsilon_0)) = \mathrm{tr}\,(f(H - \epsilon_0) - f(H_l - \epsilon_0))\,. \tag{5.7}$$

Next we will show that the right–hand side of (5.7) tends to 0 as $l \to \infty$. As the V_l are bounded in L^2 there is by Corollary 4.3

$$\begin{aligned} &\mathrm{tr}\,(f(H - \epsilon_0) - f(H_l - \epsilon_0)) \\ &\quad = \frac{1}{2\pi i} \int_{\partial K} F(z)\,\mathrm{tr}\left((z - H + \epsilon_0)^{-2} - (z - H_l + \epsilon_0)^{-2}\right) dz, \end{aligned} \tag{5.8}$$

where $K = K_{\rho,\delta(\rho)}$ with $\rho = \sigma_M - \epsilon_0$ is as in (4.1) and (4.9) respectively. N.B. K does not depend on l. We denote $\zeta = z + \epsilon_0$, decompose the difference of the resolvents

$$\begin{aligned} &(\zeta - H)^{-2} - (\zeta - H_l)^{-2} \\ &\quad = (\zeta - H)^{-2}(V - V_l)(\zeta - H_l)^{-1} + (\zeta - H)^{-1}(V - V_l)(\zeta - H_l)^{-2} \end{aligned}$$

and estimate its nuclear norm by means of Hölder's inequality and the Lemmata 3.1 and 3.4

$$\begin{aligned} &\left\|(\zeta - H)^{-2} - (\zeta - H_l)^{-2}\right\|_1 \\ &\quad \le \left\|(\zeta - H)^{-1}(V - V_l)(\zeta - H_l)^{-1}\right\|_2 \left(\left\|(\zeta - H)^{-1}\right\|_2 + \left\|(\zeta - H_l)^{-1}\right\|_2\right) \\ &\quad \le 2C_{M\delta}^3(1 + |\zeta|)^3 \left\|(\rho - \Delta)^{-1}(V - V_l)(\rho - \Delta)^{-1}\right\|_2 \left\|(\rho - \Delta)^{-1}\right\|_2 \\ &\quad \le 2C_{M\delta}^3(1 + |\zeta|)^3 \left\|(\rho - \Delta)^{-1}\right\|_2 \left\|(\rho - \Delta)^{-1/2}\right\|_4^2 \left\|(\rho - \Delta)^{-1/2}(V - V_l)(\rho - \Delta)^{-1/2}\right\| \end{aligned} \tag{5.9}$$

where $\rho = \rho_M = 1 - \sigma_M$. This decomposition ensures on the one hand the $\mathcal{B}_4$–summability of the operator $(\rho - \Delta)^{-1/2}$ (cf. Corollary 3.1) and on the other hand allows to decompose $(\rho-\Delta)^{-1/2}=(\rho-\Delta)^{-3/8}(\rho-\Delta)^{-1/8}$, into a part which maps L^2 into L^4 as

$$\operatorname{dom}(\rho-\Delta)^{3/8}\subset H^{3/4}(\Omega)\hookrightarrow L^4(\Omega)$$

(cf. e.g. [1]) and another part $(\rho-\Delta)^{-1/8}$ which is compact. By means of this decomposition we get in a first step that the sequence of operators

$$A_l=(\rho-\Delta)^{-3/8}(V-V_l)(\rho-\Delta)^{-3/8}\in\left(L^2(\Omega)\to L^2(\Omega)\right),\quad l=1,2,\dots$$

converges $A_l\rightharpoonup 0$ weakly in $\mathcal{B}(L^2(\Omega))$. Indeed there is for all $\psi,\phi\in L^2(\Omega)$

$$\begin{aligned}\langle A_l\psi,\phi\rangle &= \langle(\rho-\Delta)^{-3/8}(V-V_l)(\rho-\Delta)^{-3/8}\psi,\phi\rangle\\ &= \langle(V-V_l)(\rho-\Delta)^{-3/8}\psi,(\rho-\Delta)^{-3/8}\phi\rangle\\ &= \int_\Omega(V-V_l)(x)\,\left((\rho-\Delta)^{-3/8}\psi\right)(x)\,\left((\rho-\Delta)^{-3/8}\phi\right)(x)\,dx.\end{aligned}$$

and this tends to zero as $l\to\infty$ because $\left((\rho-\Delta)^{-3/8}\psi\right)\left((\rho-\Delta)^{-3/8}\phi\right)\in L^2(\Omega)$ and $V_l\rightharpoonup V$ weakly in $L^2(\Omega)$. Next we will show that the sequence of the operators

$$(\rho-\Delta)^{-1/2}(V-V_l)(\rho-\Delta)^{-1/2}=(\rho-\Delta)^{-1/8}A_l(\rho-\Delta)^{-1/8}$$

converges to zero in the uniform operator topology of $\mathcal{B}(L^2(\Omega))$. Otherwise there would be a sequence $\{\phi_l\}\subset L^2(\Omega)$ with $\|\phi_l\|_{L^2}=1$, $l=1,2,\dots$ such that

$$\left\|(\rho-\Delta)^{-1/8}A_l(\rho-\Delta)^{-1/8}\phi_l\right\|_{L^2}>\delta_0>0,\quad\forall l=1,2,\dots\,. \tag{5.10}$$

As the operator $(\rho-\Delta)^{-1/8}$ is compact then there would be a $\phi\in L^2(\Omega)$ and a subsequence $\{\phi_{l_j}\}_{j=1}^\infty\subset\{\phi_l\}_{l=1}^\infty$ with $(\rho-\Delta)^{-1/8}\phi_{l_j}\to\phi$ strongly in $L^2(\Omega)$. Thus we have

$$\begin{aligned}&\left\|(\rho-\Delta)^{-1/8}A_{l_j}(\rho-\Delta)^{-1/8}\phi_{l_j}\right\|_{L^2} \qquad (5.11)\\ &\le\left\|(\rho-\Delta)^{-1/8}A_{l_j}\left((\rho-\Delta)^{-1/8}\phi_{l_j}-\phi\right)\right\|_{L^2}+\left\|(\rho-\Delta)^{-1/8}A_{l_j}\phi\right\|_{L^2}.\end{aligned}$$

For every $\psi\in L^2(\Omega)$ we have $A_l\psi\rightharpoonup 0$ weakly in $L^2(\Omega)$ and because $(\rho-\Delta)^{-1/8}$ is compact, $(\rho-\Delta)^{-1/8}A_l\psi\to 0$ strongly in $L^2(\Omega)$. Thus, in particular the second term on the right–hand side of (5.11) converges towards zero as $j\to\infty$. On the other hand by the Banach–Steinhaus Theorem the operator norms $\|(\rho-\Delta)^{-1/8}A_l\|$ are bounded and as $(\rho-\Delta)^{-1/8}\phi_{l_j}\to\phi$ strongly in $L^2(\Omega)$ this implies that the first term on the right–hand side of (5.11) tends to zero. Thus we have got $\|(\rho-\Delta)^{-1/8}A_{l_j}(\rho-\Delta)^{-1/8}\|\to 0$ which is a contradiction to (5.10), hence

$$\lim_{l\to\infty}\left\|(\rho-\Delta)^{-1/2}(V-V_l)(\rho-\Delta)^{-1/2}\right\|=0. \tag{5.12}$$

Combining this result with the estimate (5.9) and (5.7), (5.8) (notice the decay properties of F as stated in (4.12)) one obtains

$$\begin{aligned} 0 &= \lim_{l\to\infty} |\mathrm{tr}\,(f(H-\epsilon_0) - f(H_l - \epsilon_0))| \\ &= \lim_{l\to\infty} |\mathrm{tr}\,(f(H_l-\epsilon_{0l}) - f(H_l - \epsilon_0))| \\ &= \lim_{l\to\infty} \sum_{j=1}^{\infty} |f(\epsilon_j(V_l)-\epsilon_{0l}) - f(\epsilon_j(V_l) - \epsilon_0)| \\ &\geq \lim_{l\to\infty} |f(\epsilon_1(V_l)-\epsilon_{0l}) - f(\epsilon_1(V_l) - \epsilon_0)| \end{aligned} \tag{5.13}$$

(recall that f is strictly decreasing and therefore all the differences $(f(\epsilon_j(V_l)-\epsilon_{0l}) - f(\epsilon_j(V_l)-\epsilon_0)$, $j=1,2,\ldots$ have the same sign). According to Theorem 2.1 the sequence $\{\epsilon_1(V_l)\}_{l=1}^{\infty}$ is bounded. hence the sequence $\{f(\epsilon_1(V_l)-\epsilon_0)\}_{l=1}^{\infty}$ is bounded and because of (5.13) $\{f(\epsilon_1(V_l)-\epsilon_{0l})\}_{l=1}^{\infty}$ is bounded too, i.e. there is an interval $[a,b]$, $0<a$, $b<\infty$ such that

$$f(\epsilon_1(V_l)-\epsilon_0) \in [a,b], \quad f(\epsilon_1(V_l)-\epsilon_{0l}) \in [a,b], \quad l=1,2,\ldots .$$

f^{-1} is strictly decreasing and continuous on $[a,b]$ because f is strictly decreasing and continuous on $\mathbf{R}$. Hence for the δ_0 from (5.6) there is a $\delta_1>0$ and for that according to (5.13) a $l_1 \in \mathbf{N}$ such that

$$|f(\epsilon_1(V_l)-\epsilon_{0l}) - f(\epsilon_1(V_l)-\epsilon_0)| < \delta_1, \quad |\epsilon_0 - \epsilon_{0l}| < \delta_0 \quad \forall l \geq l_1$$

which is a contradiction to our original assumption (5.6). □

By means of the weak compactness of $\mathcal{M}$ we get immediately

Corollary 5.1. *The Fermi level $\epsilon_0(V)$ is bounded on $\mathcal{M}$*

$$\underline{\epsilon}_{0M} \leq \epsilon_0(V) \leq \overline{\epsilon}_{0M}, \quad \forall V \in \mathcal{M}. \tag{5.14}$$

Theorem 5.2. *The Fréchet–derivative $\epsilon_0' \in (L^2(\Omega) \to L^2(\Omega))$ of the Fermi level with respect to the potential V is bounded on any M–ball $\mathcal{M}$ in $L^2(\Omega)$*

$$\|\epsilon_0'(V)\|_{L^2} \leq L_{\epsilon_0}(M) \quad \forall V \in \mathcal{M}. \tag{5.15}$$

Proof. Let be $V \in \mathcal{M}$ arbitrary, $\{\epsilon_l(V)\}_{l=1}^{\infty}$ the eigenvalues of the corresponding Schödinger operator (2.3) and $\epsilon_0(V)$, $\epsilon_0'(V)$, the Fermi level and its Fréchet–derivative at V. According to (5.5) there is

$$\|\epsilon_0'(V)\|_{L^2} = \sup_{\substack{\|W\|_{L^2}=1 \\ W\in L^2}} |\langle \epsilon_0'(V), W\rangle| = \sup_{\substack{\|W\|_{L^2}=1 \\ W\in L^2}} \left| \frac{\mathrm{tr}\,(f'(H_V-\epsilon_0(V))W)}{\mathrm{tr}\,(f'(H_V-\epsilon_0(V)))} \right| \tag{5.16}$$

We estimate the numerator in (5.16) by means of Proposition 3.3 and make use of the Dunford–integral representation (cf. Corollary 4.3) of the operator

$f'(H_V - \epsilon_0(V))W$ over the contour ∂K of the set $K = K_{\sigma_M - \bar{\epsilon}_{0M}, \delta}$ with δ as in (4.9), which can be used for all $V \in \mathcal{M}$:

$$\begin{aligned} |f'(H_V - \epsilon_0(V))W| &= \left|\operatorname{tr}\left(\frac{1}{\pi i}\int_{\partial K} F(z)\,(z - H_V + \epsilon_0(V))^{-3}\, W dz\right)\right| \\ &= \left|\frac{1}{\pi i}\int_{\partial K} F(z)\operatorname{tr}\left((z - H_V + \epsilon_0(V))^{-3}\, W\right) dz\right| \\ &\le \frac{1}{\pi}\int_{\partial K} |F(z)| \left\|(z - H_V + \epsilon_0(V))^{-3}\, W\right\|_1 dz \\ &\le \frac{c}{\pi} C^3_{M\delta} \|W\|_{L^2} \int_{\partial K} |F(z)| \left(1 + |z|^3\right) dz < \infty. \end{aligned}$$

The integral on the right–hand side is finite according to (4.12).
It remains to show that the denominator of (5.16) keeps away from zero on $\mathcal{M}$. Because of the monotonicity of f there is

$$-\sum_{l=1}^{\infty} f'(\epsilon_l(V) - \epsilon_0(V)) \ge -f'(\epsilon_1(V) - \epsilon_0(V)), \quad \forall V \in L^2(\Omega).$$

The sets $\{\epsilon_1(V)\}_{V\in\mathcal{M}}$ and $\{\epsilon_0(V)\}_{V\in\mathcal{M}}$ are bounded (cf. Theorem 2.1 and Corollary 5.1), hence there is a finite interval $[a,b]$ such that $\epsilon_1(V) - \epsilon_0(V) \in [a,b]$ for all $V \in \mathcal{M}$ and as f' is continuous there is a $s_M \in [a,b]$ with

$$0 > f'(s_M) = \max_{s\in[a,b]} f'(s) \ge \sup_{V\in\mathcal{M}} f'(\epsilon_1(V) - \epsilon_0(V)).$$

Thus we have got that (5.16) is uniformly bounded for all $V \in \mathcal{M}$. □

Corollary 5.2. *The mapping $\epsilon_0 \in (\mathcal{M} \to \mathbf{R})$ is Lipschitz–continuous with the constant from Theorem 5.2*

$$|\epsilon_0(V_1) - \epsilon_0(V_2| \le L_{\epsilon_0}(M)\|V_1 - V_2\|_{L^2}, \quad \forall V_1, V_2 \in \mathcal{M}. \tag{5.17}$$

6. The Electron Density $n = n(V)$

6.1. Boundedness. For every $V \in L^2(\Omega)$ the electron density $n = n(V)$ is defined by

$$n(V)(x) = \sum_{l=1}^{\infty} f(\epsilon_l(V) - \epsilon_0(V))\,|\psi_l(V)(x)|^2 \quad x \in \Omega\,, \tag{6.1}$$

where $\{\epsilon_l(V)\}_{l=1}^{\infty}$ and $\{\psi_l(V)\}_{l=1}^{\infty}$ are the eigenvalues in increasing order (counting multiplicity) and the corresponding eigenfunctions of the Schrödinger operator (2.3) and $\epsilon_0 = \epsilon_0(V)$ is the Fermi level. The series

$$\sum_{l=1}^{\infty} f(\epsilon_l(V) - \epsilon_0(V)) = \operatorname{tr}\left(f(H_V - \epsilon_0(V)\right)$$

converges according to Theorem 4.2. Hence, $n(V) \in L^1(\Omega)$.

Proposition 6.1. *For all potentials $V \in L^2(\Omega)$ there is $n(V) \in L^\infty(\Omega)$ and the defining series* (6.1) *converges uniformly for all $x \in \overline{\Omega}$. For every $M > 0$ we may notice*

$$\sup_{V\in\mathcal{M}} \|n(V)\|_{L^\infty} < \infty, \tag{6.2}$$

where $\mathcal{M}$ denotes the closed M-ball in $L^2(\Omega)$.

Proof. Let be $V \in \mathcal{M}$ arbitrary, $\{\epsilon_l(V)\}_{l=1}^{\infty}$ the eigenvalues (counting multiplicity) of the corresponding Schödinger operator (2.3) and $\epsilon_0(V)$ the Fermi level. We estimate (6.1) making use of the Dunford–integral representation (cf. Corollary 4.3) of the operator $f(H_V - \epsilon_0(V))$ over the contour ∂K of the set $K = K_{\sigma_M,\delta}$ with δ as in (4.9), thereby using (3.12), Lemma 3.4, Proposition 3.1 and Corollary 5.1 and abbreviating $\epsilon_l = \epsilon_l(V)$, $l = 0, 1, 2, \ldots$:

$$
\begin{aligned}
\|n(V)\|_{L^\infty} &\le \frac{c^2}{C_M^2} \sum_{l=1}^{\infty} f(\epsilon_l - \epsilon_0)(\rho_M + \epsilon_l)^2 \\
&= c_0(M)\,\mathrm{tr}\left(f(H_V - \epsilon_0)(\rho_M + H_V)^2\right) \\
&= c_0(M)\,\mathrm{tr}\left(\frac{3}{\pi i}\int_{\partial K} f^{-3}(z)(z - H_V + \epsilon_0)^{-4}\,dz\,(\rho_M + H_V)^2\right) \\
&\le c_1(M)\int_{\partial K} \left|f^{-3}(z)\right| \left\|(z - H_V + \epsilon_0)^{-4}(\rho_M + H_V)^2\right\|_1 dz \\
&= c_1(M)\int_{\partial K} \left|f^{-3}(z)\right| \left\|(z - H_V + \epsilon_0)^{-4}\left((\rho_M + \epsilon_0 + z) - (z - H_V + \epsilon_0)\right)^2\right\|_1 dz \\
&= c_1(M)\int_{\partial K} \left|f^{-3}(z)\right| \Big\|(\rho_M + \epsilon_0 + z)^2 (z - H_V + \epsilon_0)^{-4} \\
&\qquad - 2(\rho_M + \epsilon_0 + z)(z - H_V + \epsilon_0)^{-3} + (z - H_V + \epsilon_0)^{-2}\Big\|_1 dz \\
&\le c_1(M)\int_{\partial K} \left|f^{-3}(z)\right| \Big\{|\rho_M + \epsilon_0 + z|^2\, C_{M\delta}^4\left(1 + |z + \epsilon_0|^4\right) \\
&\qquad + 2\,|\rho_M + \epsilon_0 + z|\, C_{M\delta}^3\left(1 + |z + \epsilon_0|^3\right) + C_{M\delta}^2\left(1 + |z + \epsilon_0|^2\right)\Big\}\, dz \\
&\le c_2(M)\int_{\partial K} \left|f^{-3}(z)\right| \left(1 + |z|^6\right) dz \;<\; \infty.
\end{aligned}
$$

The integral on the right–hand side is finite according to (4.12) and the whole right–hand side does not depend any more on V. □

6.2. Potentiality. We will prove that the electron–density operator

$$
n \in \left(L^2(\Omega) \to L^2(\Omega)\right) \tag{6.3}
$$

which maps an electrostatic potential $V \in L^2(\Omega)$ onto the corresponding electron density (6.1) is a potential–operator.

Lemma 6.1. *Let be H_V the Schrödinger operator* (2.3) *with the potential V, $\epsilon_0(V)$ the corresponding Fermi-level* (5.1)*, $U \in L^2(\Omega)$ arbitrary but fixed and $f^{(-j)}$, $j = 0, 1$ the primitive* (4.8) *of a distribution function f with* (4.10),(4.11) *or this function itself. The function*

$$
\mathcal{F} \in \left(L^2(\Omega) \to \mathcal{B}_1\right) \quad \mathcal{F}(V) = U\, f^{(-j)}(H_V - \epsilon_0(V)) \tag{6.4}
$$

is Fréchet differentiable for every $V \in L^2(\Omega)$ *and the derivative* $\mathcal{F}'(V) \in \mathcal{B}(L^2(\Omega), \mathcal{B}_1)$ *is given by*

$$\mathcal{F}'(V)[W] = \frac{U}{2\pi i}\int_\Gamma f^{(-j-1)}(z)\left(R^2(z)WR(z) + R(z)WR^2(z)\right)dz$$
$$- \frac{\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)W\right)}{\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)\right)}\, Uf^{(1-j)}\left(H_V - \epsilon_0(V)\right) \quad \forall W \in L^2(\Omega), \quad (6.5)$$

where $R = R(z) = (z - H_V + \epsilon_0(V))^{-1}$ *and* Γ *is any* $K_{\rho,\delta(\rho)}$*-admissible path with positive distance to the half-axis* $[\rho, \infty)$. $K = K_{\rho,\delta(\rho)}$ *is the set* (4.1) *with* $\rho = \sigma_M - \bar{\epsilon}_{0M}$ *and* $M > \|V\|_{L^2}$, σ_M *and* $\bar{\epsilon}_{0M}$ *being the lower bound* (2.4) *of the spectrum and the upper bound* (5.14) *of the Fermi level, respectively.*

Proof. In the same way as in the proof of Theorem 4.3 one can show that $\mathcal{F}'(V)$ is indeed from $\mathcal{B}(L^2(\Omega), \mathcal{B}_1)$. Now without loss of generality let be $W \in L^2(\Omega)$ such that $\|V + W\|_{L^2} \le M$. Then

$$\mathcal{F}(V+W) - \mathcal{F}(V) = U\, f^{(-j)}\left(H_{V+W} - \epsilon_0(V+W)\right) - U\, f^{(-j)}\left(H_V - \epsilon_0(V)\right)$$
$$= \frac{U}{2\pi i}\int_\Gamma f^{(-j-1)}(z)\left((z + \epsilon_0(V+W) - H_V - W)^{-2} - (z + \epsilon_0(V) - H_V)^{-2}\right) dz\,.$$

N.B. the requirements on the contour Γ in the lemma serve for both arguments $H_{V+W} - \epsilon_0(V+W)$ and $H_V - \epsilon_0(V)$ of the function $f^{(-j)}$. Now we decompose the difference of the resolvent–squares (cf. §3.3) under the integral

$$R_W^2 - R^2 = R^2WR + RWR^2 - 2\langle\epsilon_0'(V), W\rangle R^3$$
$$- 2\omega_\epsilon(V,W)R^3 + RR_W(WR)^2 + R_W(WR)^2R + (R_WWR)^2$$
$$+ \left(\langle\epsilon_0'(V), W\rangle^2 + \omega_\epsilon^2(V,W)\right)\left(RR_WR^2 + R_WR^3 + (R_WR)^2\right) \quad (6.6)$$

where $R_W = R_W(z) = (z - (H_V - \epsilon_0(V) + W - \langle\epsilon_0'(V), W\rangle - \omega_\epsilon(V,W)))^{-1}$ and $\epsilon_0'(V)$ is the Fréchet–derivative (5.5) of the Fermi level at V. By $\omega_\epsilon(V,W)$ we denote the remainder in the linear expansion $\epsilon_0(V+W) = \epsilon_0(V) + \langle\epsilon_0'(V), W\rangle + \omega_\epsilon(V,W)$. The first three terms in (6.6) are the contribution to the derivative. According to (5.5) and Corollary 4.3 there is indeed for all $W \in L^2(\Omega)$

$$\frac{2\langle\epsilon_0'(V), W\rangle}{2\pi i}\int_\Gamma f^{(-j-1)}(z)R^3(z)\,dz = \frac{\operatorname{tr}(f'(H_V - \epsilon_0(V))W)}{\operatorname{tr}(f'(H_V - \epsilon_0(V)))} f^{(1-j)}\left(H_V - \epsilon_0(V)\right).$$

For the remainder of the linear expansion of $\mathcal{F}(V+W)$ at V we get

$$\omega(V,W) = \mathcal{F}(V+W) - \mathcal{F}(V) - \mathcal{F}'(V)[W]$$
$$= \frac{U}{2\pi i}\int_\Gamma f^{(-j-1)}(z)\left(-2\omega_\epsilon(V,W)R^3 + RR_W(WR)^2 + R_W(WR)^2R + (R_WWR)^2\right.$$
$$\left. + \left(\langle\epsilon_0'(V), W\rangle^2 + \omega_\epsilon^2(V,W)\right)\left(RR_WR^2 + R_WR^3 + (R_WR)^2\right)\right) dz.$$

By means of Proposition 3.2 and 3.3 we can estimate the nuclear norm of $\omega(V,W)$

$$\|\omega(V,W)\|_1 \le \tilde{c}\, \|U\|_{L^2}\left(C_{M\delta}^3\, o(\|W\|_{L^2})\int_K \left|f^{(-j-1)}(z)\right|\left(1 + |z|^3\right)dz\right.$$
$$\left. + C_{M\delta}^4\left(\|W\|_{L^2}^2 + \|\epsilon_0'(V)\|_{L^2}^2\|W\|_{L^2}^2 + o(\|W\|_{L^2}^2)\right)\int_K \left|f^{(-j-1)}(z)\right|\left(1 + |z|^4\right)dz\right).$$

The integrals on the right–hand side are finite according to (4.12). Thus, $\|\omega(V,W)\|_1$ is indeed a $o(\|W\|_{L^2})$. $\square$

Theorem 6.1. *Let be $H = H_V$ the Schrödinger operator* (2.3) *with the potential V, $\epsilon_0 = \epsilon_0(V)$ the corresponding Fermi–level* (5.1) *and f a distribution function with* (4.10),(4.11). *There is the following representation of the electron–density operator*

$$\langle n(V), W\rangle = \int_\Omega W(x)n(V)(x)dx = \operatorname{tr}\left(f(H_V - \epsilon_0(V))W\right), \quad \forall V, W \in L^2(\Omega). \tag{6.7}$$

Proof. We calculate the trace of the operator $f(H-\epsilon_0)W$ with respect to the eigenfunctions $\{\psi_l\}_{l=1}^\infty$ of the Schrödinger operator H and use its spectral decomposition $H = \sum_{l=1}^\infty \epsilon_l\,(\cdot,\psi_l)_{L^2}\,\psi_l$. As H is self–adjoint and f is real–valued for real arguments the operator $f(H-\epsilon_0)$ is self–adjoint. Thus,

$$\begin{aligned}
\operatorname{tr}(f(H-\epsilon_0)W) &= \sum_{l=1}^\infty (f(H-\epsilon_0)W\psi_l,\psi_l)_{L^2} = \sum_{l=1}^\infty (W\psi_l, f(H-\epsilon_0)\psi_l)_{L^2} \\
&= \sum_{l=1}^\infty \left(W\psi_l\,,\, \sum_{j=1}^\infty f(\epsilon_j-\epsilon_0)\,(\psi_l,\psi_j)_{L^2}\,\psi_j\right)_{L^2} = \sum_{l=1}^\infty (W\psi_l, f(\epsilon_l-\epsilon_0)\psi_l)_{L^2} \\
&= \sum_{l=1}^\infty \int_\Omega W(x)f(\epsilon_l-\epsilon_0)|\psi_l(x)|^2dx = \int_\Omega W(x)\sum_{l=1}^\infty f(\epsilon_l-\epsilon_0)|\psi_l(x)|^2dx = \langle n(V),W\rangle
\end{aligned}$$

for all $W \in L^2(\Omega)$. $\square$

Theorem 6.2. *Let be H_V the Schrödinger operator* (2.3) *with the potential V and $\epsilon_0(V)$ the corresponding Fermi–level* (5.1). *The functional $\phi \in (L^2(\Omega) \to \mathbf{R})$*

$$\phi(V) = \bar{n}_D\,\epsilon_0(V) + \operatorname{tr}\left(F(H_V - \epsilon_0(V))\right), \quad V \in L^2(\Omega) \tag{6.8}$$

is Fréchet differentiable for every $V \in L^2(\Omega)$ and the derivative $\phi'(V) \in (L^2(\Omega))^* \equiv L^2(\Omega)$ is the electron density $\phi'(V) = n(V)$.

Proof. Since the trace is a continuous linear functional on $\mathcal{B}_1$ one obtains by means of Lemma 6.1 (take $j=1$ and $U \equiv 1$)

$$\begin{aligned}
\langle \phi'(V), W\rangle &= \bar{n}_D\langle \epsilon_0'(V), W\rangle + \operatorname{tr}\left(\mathcal{F}'(V)[W]\right) \\
&= \operatorname{tr}\left(\frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\left(R^2(z)WR(z) + R(z)WR^2(z)\right)dz\right) \quad \forall W \in L^2(\Omega).
\end{aligned}$$

N.B. according to (5.5) and (5.1) the trace of the second term in (6.5) is just $-\bar{n}_D\langle\epsilon_0'(V),W\rangle$. In the same way as in the proof of Theorem 4.4 one can show

$$\operatorname{tr}\left(\frac{1}{2\pi i}\int_\Gamma f^{(-2)}(z)\left(R^2(z)WR(z) + R(z)WR^2(z)\right)dz\right) = \operatorname{tr}\left(f(H_V - \epsilon_0(V))W\right)$$

for all $W \in L^2(\Omega)$. Now the assertion follows with Theorem 6.1. $\square$

6.3. Fréchet differentiability.

Theorem 6.3. *The electron–density operator* (6.3) *is Fréchet differentiable for every* $V \in L^2(\Omega)$ *and the derivative* $n'(V) \in \mathcal{B}(L^2(\Omega))$ *is given by*

$$\langle n'(V)[W], U\rangle = \operatorname{tr}\left(\frac{U}{2\pi i}\int_\Gamma F(z)\left(R^2(z)WR(z) + R(z)WR^2(z)\right)dz\right) - \frac{\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)W\right)\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)U\right)}{\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)\right)} \quad \forall U, W \in L^2(\Omega), \tag{6.9}$$

where H_V *is the Schrödinger operator* (2.3) *with the potential* V, $\epsilon_0(V)$ *the corresponding Fermi–level* (5.1) *and* R *and* Γ *are as in Lemma* 6.1.

Proof. The assertion follows from Theorem 6.1 and Lemma 6.1 where we take $j = 0$ and get

$$\langle n'(V)[W], U\rangle = \operatorname{tr}\left(\mathcal{F}'(V)[W]\right) \quad \forall U, W \in L^2(\Omega),$$

with $\mathcal{F}(V) = Uf(H_V - \epsilon_0(V))$. □

Remark 6.1. If the directions U and W coincide (6.9) can be written in a more condensed form, viz.

$$\langle n'(V)[W], W\rangle = \operatorname{tr}\left(\frac{1}{2\pi i}\int_\Gamma f(z)\left(WR(z)\right)^2 dz\right) - \frac{\left(\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)W\right)\right)^2}{\operatorname{tr}\left(f'\left(H_V - \epsilon_0(V)\right)\right)}$$

for all $W \in L^2(\Omega)$. Indeed there is

$$WR^2(z)WR(z) + WR(z)WR^2(z) = -\frac{d}{dz}\left(WR(z)\right)^2$$

and observing the decay properties (4.12) of F one can integrate by parts

$$-\int_\Gamma F(z)\frac{d}{dz}\left(WR(z)\right)^2 dz = \int_\Gamma f(z)\left(WR(z)\right)^2 dz.$$

N.B. we cannot use this formula for the monotonicity–proof, as NIER [11] did, since we do not have the nuclearity of the operators $(WR(z))^2$ for arbitrary potentials V from $L^2(\Omega)$.

6.4. Bounded Lipschitz–continuity.

Lemma 6.2. *The Fréchet-derivative* $n' \in (L^2(\Omega) \to \mathcal{B}(L^2))$ *of the electron-density operator* (6.3) *with respect to the potential* V *is bounded on* $\mathcal{M}$

$$\|n'(V)\| \le L_n(M) \quad \forall V \in \mathcal{M} \tag{6.10}$$

for every $M > 0$, $\mathcal{M}$ *being the* M*–ball in* $L^2(\Omega)$.

Proof. Let be $V \in \mathcal{M}$, $H = H_V$ the Schrödinger operator (2.3) with the potential V, $\epsilon_0 = \epsilon_0(V)$ the corresponding Fermi–level (5.1), $R = R(z) = (z - H + \epsilon_0)^{-1}$, $K = K_{\rho,\delta(\rho)}$ the set (4.1) with $\rho = \sigma_M - \bar{\epsilon}_{0M}$, σ_M and $\bar{\epsilon}_{0M}$ being the lower bound (2.4) of the spectrum and the upper bound (5.14) of the Fermi level, respectively. We calculate

$$\|n'(V)\| = \sup_{\substack{U,W \in L^2 \\ \|U\|_{L^2} = \|W\|_{L^2} = 1}} \langle n'(V)[W], U\rangle$$

by means of Theorem 6.3 and get with (5.5) and Theorem 5.2

$$\begin{aligned}\langle n'(V)[W],U\rangle &\le \frac{1}{2\pi}\int_{\partial K}|F(z)|\left\|UR^2(z)WR(z)+UR(z)WR^2(z)\right\|_1 dz \\ &+ L_{\epsilon_0}(M)\|W\|_{L^2}\|f'(H-\epsilon_0)U\|_1 \quad \forall U,W\in L^2(\Omega).\end{aligned}$$

As for the second term on the right–hand side we may observe via Corollary 4.3

$$\|f'(H-\epsilon_0)U\|_1 \le \frac{1}{\pi}\int_{\partial K}|F(z)|\left\|UR^3(z)\right\|_1 dz \quad \forall U\in L^2(\Omega).$$

We estimate the nuclear norms in the preceding formulas by means of Hölder's inequality, Proposition 3.2 and Proposition 3.3 and get for all $U,W\in L^2(\Omega)$

$$\langle n'(V)[W],U\rangle \le \frac{c}{\pi}C^3_{M\delta}\left(1+L_{\epsilon_0}(M)\right)\|U\|_{L^2}\|W\|_{L^2}\int_K |F(z)|\left(1+|z|^3\right)dz$$

The integral on the right–hand side is finite according to (4.12). □

From Lemma 6.2 immediately follows

Theorem 6.4. *The electron–density operator* (6.3) *is bounded Lipschitzian, i.e. for each* $M>0$ *there is a* $L_n(M)$ *such that*

$$\|n(V_2)-n(V_1)\|_{L^2}\le L_n(M)\,\|V_2-V_1\|_{L^2},\quad \forall V_1,V_2\in\mathcal{M}. \tag{6.11}$$

6.5. Monotonicity.

Theorem 6.5. *The negative electron–density operator* (6.3) *is monotone:*

$$\langle n(V_2)-n(V_1),V_1-V_2\rangle \ge 0 \quad \forall V_1,\ V_2\in L^2(\Omega). \tag{6.12}$$

Proof. We will show that

$$\langle n'(V)[W],W\rangle \le 0 \quad \forall V,W\in L^2(\Omega). \tag{6.13}$$

This implies the monotonicity of the operator $-n$ (cf. [3], ch. III, Lemma 1.1). According to Theorem 6.3 there is for all $W\in L^2(\Omega)$ with R and Γ as in Lemma 6.1

$$\langle n'(V)[W],W\rangle = \frac{1}{\pi i}\int_\Gamma F(z)\,\mathrm{tr}\left(R(z)\,(WR(z))^2\right)dz - \frac{\left(\mathrm{tr}\left(f'\left(H_V-\epsilon_0(V)\right)W\right)\right)^2}{\mathrm{tr}\left(f'\left(H_V-\epsilon_0(V)\right)\right)}$$

Let us calculate the trace of $R(WR)^2$ with respect to the eigenfunctions $\{\psi_l\}_{l=1}^\infty$ of the Schrödinger operator H_V:

$$\begin{aligned}\mathrm{tr}\left(R(WR)^2\right) &= \sum_{l=1}^\infty\left(WRWR^2\psi_l,\psi_l\right)_{L^2} = \sum_{l=1}^\infty\left(R^2(z)\psi_l, WR(\bar z)W\psi_l\right)_{L^2} \\ &= \sum_{l=1}^\infty\frac{(R(z)W\psi_l,W\psi_l)_{L^2}}{(z-\epsilon_l+\epsilon_0)^2} = \sum_{j,k,l=1}^\infty\frac{(R(z)\psi_j,\psi_k)_{L^2}(W\psi_l,\psi_j)_{L^2}(\psi_k,W\psi_l)_{L^2}}{(z-\epsilon_l+\epsilon_0)^2} \\ &= \sum_{k,l=1}^\infty\frac{(W\psi_l,\psi_k)_{L^2}(\psi_k,W\psi_l)_{L^2}}{(z-\epsilon_l+\epsilon_0)^2(z-\epsilon_k+\epsilon_0)} = \sum_{k,l=1}^\infty\frac{|(W\psi_l,\psi_k)_{L^2}|^2}{(z-\epsilon_l+\epsilon_0)^2(z-\epsilon_k+\epsilon_0)}.\end{aligned}$$

By means of Lemma 4.1 and Corollary 4.1 one can evaluate the contour integral

$$\begin{aligned} F_{k,l} &= \frac{1}{\pi i}\int_\Gamma \frac{F(z)}{(z-\epsilon_l+\epsilon_0)^2(z-\epsilon_k+\epsilon_0)} \\ &= \begin{cases} f'(\epsilon_l-\epsilon_0) & \text{if } \epsilon_l=\epsilon_k \\ \frac{2}{(\epsilon_l-\epsilon_k)^2}\left(F(\epsilon_k-\epsilon_0)-F(\epsilon_l-\epsilon_0)-f(\epsilon_l-\epsilon_0)(\epsilon_k-\epsilon_l)\right) & \text{if } \epsilon_l\neq\epsilon_k \end{cases} \end{aligned}$$

which is always negative as the distribution function is strictly decreasing. Thus,

$$\begin{aligned} &\operatorname{tr}\left(f'\left(H_V-\epsilon_0(V)\right)\right)\ \langle n'(V)[W],W\rangle \\ &\quad = \frac{1}{2}\sum_{k,l=1}^{\infty} f'(\epsilon_k-\epsilon_0)\,f'(\epsilon_l-\epsilon_0)\left((W\psi_k,\psi_k)_{L^2}-(W\psi_l,\psi_l)_{L^2}\right)^2 \\ &\qquad + \operatorname{tr}\left(f'\left(H_V-\epsilon_0(V)\right)\right)\left(\sum_{\substack{k,l=1\\k\neq l}}^{\infty} F_{kl}\left|(W\psi_l,\psi_k)_{L^2}\right|^2\right). \end{aligned}$$

This expression is always nonnegative and vanishes iff W is a constant a.e. in Ω. As $\operatorname{tr}\left(f'\left(H_V-\epsilon_0(V)\right)\right)$ is strictly negative this implies (6.13). □

Corollary 6.1. *The restriction of the negative electron–density operator* (6.3) *on the space* $H_0^1(\Omega)$ *is strictly monotone:*

$$\langle n(V_2)-n(V_1),V_1-V_2\rangle > 0 \quad \forall V_1\neq V_2\in H_0^1(\Omega). \tag{6.14}$$

7. Existence, uniqueness and regularity

Theorem 7.1. *For every* $n_D\in L^2(\Omega)$ *the Schrödinger–Poisson operator* (1.6) *is a strongly monotone*

$$\langle A(V_2)-A(V_1),V_2-V_1\rangle > \|V_2-V_1\|^2_{H_0^1} \quad \forall V_1,V_2\in H_0^1(\Omega) \tag{7.1}$$

and bounded Lipschitz–continuous

$$\begin{aligned} &\|A(V_2)-A(V_1)\|_{H^{-1}} \le (1+c\,L_n(M))\,\|V_2-V_1\|_{H_0^1} \\ &\qquad\qquad \forall V_j\in H_0^1(\Omega) \text{ with } \|V_0+V_j\|_{L^2}\le M,\ j=1,2 \end{aligned} \tag{7.2}$$

potential operator. Its inverse $A^{-1}\in(H^{-1}(\Omega)\to H_0^1(\Omega))$ *is a strictly monotone and Lipschitz–continuous*

$$\|A^{-1}(n_2)-A^{-1}(n_1)\|_{H_0^1} < \|n_2-n_1\|_{H^{-1}} \quad \forall n_1,n_2\in H^{-1}(\Omega) \tag{7.3}$$

potential operator. — In (7.2) $L_n(M)$ *is the constant from* (6.11) *and* c *is the product of the embedding constants* $c_{L^2\hookrightarrow H^{-1}}$ *and* $c_{H_0^1\hookrightarrow L^2}$.

Proof. The Schrödinger–Poisson operator (1.6) is the difference

$$A(V)=JV-n(V_0+V)$$

of the duality mapping (1.10) and the electron–density operator (6.3). The duality mapping J is strongly monotone and Lipschitz–continuous with both constants 1. Hence (7.1) and (7.2) follow from Corollary 6.1 and Theorem 6.4, respectively. The duality mapping is also a potential operator and so is n and thus A according to Theorem 6.2. Now a well known theorem (cf. [3] ch. III, Th. 4.9) provides the existence, potentiality and strict monotonicity of A^{-1}. Direct calculation shows the Lipschitz–continuity of A^{-1} (cf. [3] ch. III, Cor. 2.3) . $\square$

According to Theorem 7.1 the Schrödinger–Poisson equation (1.5) has exactly one solution $V \in H_0^1(\Omega)$ for every right–hand side from $H^{-1}(\Omega)$. As we assume $n_D \in L^2(\Omega)$ we can get better regularity of the solution $V = J^{-1}(n(V_0+V) - n_D)$.

Theorem 7.2. *For every $n_D \in L^2(\Omega)$ the solution of the Schrödinger–Poisson equation* (1.5) *belongs to the space $H^2(\Omega) \cap H_0^1(\Omega)$.*

The proof follows from assumption (1.14). By embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ one obtains

Corollary 7.1. *For every $n_D \in L^2(\Omega)$ the solution of the Schrödinger–Poisson equation* (1.5) *belongs to the space $L^\infty(\Omega)$.*

8. Iteration scheme

Let be $V_1 \in H_0^1$ an arbitrary starting point and $a > 0$ any positive real number. We define the iteration sequence $\{V_l\}_{l=1}^\infty \subset H_0^1(\Omega)$ by

$$V_{l+1} = (1-t_l)V_l + t_l J^{-1}\left(n(V_0+V_l) - n_D\right) \qquad l = 1,2,\dots,$$

$$t_l = \min\left\{1, \frac{2}{a+\mu_l}\right\} \qquad \mu_l = \mu\left(\|V_l\|_{H_0^1} + \|JV_l - n(V_0+V_l) + n_D\|_{H^{-1}}\right) \tag{8.1}$$

where μ is an increasing function with

$$\|A(U) - A(V)\|_{H^{-1}} \leq \mu\left(\max\left\{\|U\|_{H_0^1}, \|V\|_{H_0^1}\right\}\right)\|U-V\|_{H_0^1}, \quad \forall U,V \in H_0^1.$$

(7.2) provides such a function μ. According to [3] ch. III, Th. 4.2, Rem. 4.12 we have

Theorem 8.1. *The sequence* (8.1) *converges strongly in $H_0^1(\Omega)$ towards the solution V of the Schrödinger–Poisson equation* (1.5).

Remark 8.1. The dynamical step size in (8.1) can be replaced by a constant $t_l = t$ and any smaller positive value can be used just as well (cf. [3] ch. III, Rem. 4.11). — Theorem 8.1 implies that the sequence $\{V_l\}_{l=1}^\infty$ is bounded in L^2. So in the following we can choose a finite M such that

$$\|V_0 + V_l\|_{L^2} \leq M, \quad l = 1,2,\dots. \tag{8.2}$$

Thus we have uniform constants for all members of the iteration sequence and the solution.

Ultimately we are interested in uniform convergence of the sequence (8.1). By means of assumption (1.14) we may notice

Lemma 8.1. *For every starting point $V_1 \in H^2(\Omega) \cap H_0^1(\Omega)$ the iteration sequence* (8.1) *belongs to the spaces $H_0^1(\Omega)$, $H^2(\Omega)$ and $L^\infty(\Omega)$.*

Theorem 8.2. *Let be $V_1 \in H^2(\Omega) \cap H_0^1(\Omega)$. Then the iteration sequence* (8.1) *converges **weakly** in $H^2(\Omega)$ towards the solution V of the Schrödinger–Poisson equation* (1.5).

Proof. In §6.4 we have proved that the electron–density operator is bounded Lipschitzian. Hence the H_0^1–convergence $V_l \to V$ of the iteration sequence (8.1) implies

$$n(V_l) \to n(V) \quad \text{in } L^2(\Omega).$$

As $J^{-1} \in \mathcal{B}(L^2, H^2)$ (cf. assumption (1.14)) we have

$$J^{-1}(n(V_l)) \to J^{-1}(n(V)) \quad \text{in } H^2(\Omega),$$

i.e. the sequence $\{J^{-1}(n(V_l))\}_{l=1}^{\infty}$ is bounded in H^2:

$$\left\| J^{-1}(n(V_l)) \right\|_{H^2} \le K, \quad l = 1, 2, \dots .$$

Now from the definition (8.1) of the iteration sequence we may deduce

$$\begin{aligned} \|V_{l+1}\|_{H^2} &\le (1-t)\|V_l\|_{H^2} + tK \le (1-t)^l \|V_1\|_{H^2} + tK \sum_{\nu=0}^{l-1} (1-t)^\nu \\ &\le \|V_1\|_{H^2} + \frac{tK}{1-t} \qquad (\text{N.B. } 0 < t < 1). \end{aligned}$$

Thus we have got that the iteration sequence (8.1) is bounded in the space $H^2(\Omega)$. As $H^2(\Omega)$ is reflexive $\{V_l\}_{l=1}^{\infty}$ is also weakly compact. Now the assertion follows from the already established H_0^1–convergence of the whole sequence $\{V_l\}_{l=1}^{\infty}$. □

Corollary 8.1. *Let be $V_1 \in H^2(\Omega) \cap H_0^1(\Omega)$. Then the iteration sequence* (8.1) *converges* ***strongly*** *towards the solution V of the Schrödinger–Poisson equation* (1.5) *in every space to which $H^2(\Omega) \cap H_0^1(\Omega)$ has a compact embedding, especially in $L^\infty(\Omega)$.*

Let be $H_l = -\Delta + V_0 + V_l$ the Schrödinger operator (2.3) corresponding to the potential $V_0 + V_l$ which the iteration sequence (8.1) provides and $\sigma(H_l)$ the spectrum of H_l. There is (cf. [9] ch. V, Th. 4.10)

$$\begin{aligned} \operatorname{dist}(\sigma(H_{l+1}), \sigma(H_l)) &\le \|H_{l+1} - H_l\| = \|V_{l+1} - V_l\|_{L^\infty}, \\ \operatorname{dist}(\sigma(H_V), \sigma(H_l)) &\le \|H_V - H_l\| = \|V - V_l\|_{L^\infty}, \end{aligned}$$

V being the solution of the Schrödinger–Poisson equation (1.5) and H_V the corresponding Schrödinger operator (2.3).

The Schrödinger operators (2.3) are operators with compact resolvent (cf. Proposition 3.1). Hence, their spectrum consists entirely of isolated eigenvalues with finite multiplicity. Thus, for each $\lambda \in \sigma(H_V)$, V being again the solution of the Schrödinger–Poisson equation (1.5), there is an index $l(\lambda)$, such that

$$d_{isol.} = \operatorname{dist}(\lambda, \sigma(H_V) \setminus \{\lambda\}) > 2\, \|V_l - V\|_{L^\infty}, \quad \forall l \ge l(\lambda).$$

Let be m the multiplicity of $\lambda \in \sigma(H_V)$. Then for each $l \ge l(\lambda)$, H_l has exactly m repeated eigenvalues in the interval $\left(\lambda - \frac{d_{isol.}}{2}, \lambda + \frac{d_{isol.}}{2}\right)$ and at most m repeated eigenvalues in the interval $(\lambda - \|V - V_l\|_{L^\infty}, \lambda + \|V - V_l\|_{L^\infty})$ (cf. [9] V.4.3 and take there $T = H_V$, $S = H_l$, $a = \|V - V_l\|_{L^\infty}$, $b = 0$).

A Note on the Discretization of a Stationary Schrödinger–Poisson System (by G. Albinus)

Abstract: Recently it has been observed that the stationary Schrödinger-Poisson system is a variational problem with a strongly monotone potential operator. In this note a way of discretization is described such that the discretized problem is also a variational problem with a boundedly Lipschitz continuous strongly monotone potential operator. These properties guarantee the unique solvability of the discrete problem as well as the convergence of the iteration method of the steepest gradient.

Key words: stationary Schrödinger–Poisson system, discretization of the Schrödinger–Poisson system, monotone potential operators, iterative methods

1991 Mathematics Subject Classification: 65N30, 47H05, 47A60, 47H17, 49M07, 65N22, 81V45, 82B05

1. Introduction

The atom is a 'classical' example of a quantum mechanical system of some electrons which may be described by a stationary Schrödinger–Poisson system. The atom is considered as a system which consists of a fixed nucleus and a number of electrons around the nucleus. If the interaction of the electrons among another is neglected the single electrons 'see' the nucleus as an Hamilton operator H_0 in a Hilbert space, let us say $L_2(R^3)$. The Hamilton operator is positive definite and has real eigenvalues $\epsilon_1 \leq \epsilon_2 \leq ...$ and eigenstates $\psi_l, l = 1, 2, ...$ If the Pauli principle is regarded in a rudimentary way the nucleus of a stable atom with K protons binds K electrons in the K lowest states. A better description may be expected if the electrostatic interaction of the electrons is also considered. Roughly speaking the stationary Schrödinger–Poisson system for the stable atom with K electrons consists in an eigenvalue problem

$$(H_0 + V)\psi_l = \epsilon_l\psi_l \qquad (l = 1, 2, ..., K)$$

for a Schrödinger operator with an unknown potential V which is defined by the sought eigenfunctions,

$$V(x) = \frac{a}{4\pi}\int\sum|\psi_l(y)|^2\frac{dy}{|x-y|}.$$

Advances in the semiconductor technology are another source of interest in stationary Schrödinger–Poisson systems. In this case one may consider a rather small (part of an) electronic device which consists of a semiconductor material with a fixed positive doping profile such that the equilibrium of the system of the crystal electrons in the conductive band should be described by quantum mechanics and statistics. The lattice together with the exterior electrostatic conditions are represented by an undisturbed Hamilton operator H_0 which operates on the states of single crystal electrons. Let us regard again the electrostatic interaction of electrons. Thus we ask for the eigenvalues ϵ_l and the eigenfunctions ψ_l of an Hamilton operator $H = H_0 + V$ in $L_2(\Omega)$, the unknown potential V of which is determined by the eigenvalues and eigenfunctions in the following way.

With an energy distribution function f and with the fixed density $D \geq 0$ of the doping profile the Fermi level φ_D is defined by the condition

$$\int D = \sum_l f(\epsilon_l - \varphi_D) ,$$

which turns out to be just the supposed charge neutrality of the system. Now the electron density N is defined by

$$N_V(x) = \sum_l f(\epsilon_l - \varphi_D)|\psi_l(x)|^2 .$$

If the electron charge is -1 and if H_0 does not contain the electrostatic interaction between the electrons and the doping profile, then the potential V of the electrons due to the electric charge is the solution of a boundary value problem for the Poisson equation

$$-\nabla \cdot (\epsilon \nabla V) = N_V - D$$

under homogeneous boundary conditions. F. Nier [11] has observed that this nonlinear problem is a variational problem with a strongly monotone potential operator. H.-C. Kaiser and J. Rehberg (cf. this preprint) have shown that this operator is also boundedly Lipschitz continuous in $L_2(\Omega)$.

In this note, answering a question of H. Gajewski, we will show that the nice structure of the nonlinear problem can be preserved under discretization. If one is going to discretize the stationary Schrödinger–Poisson system, one should take regard to the fact that the wave functions ψ, the potentials V and the electron densities N are all described by functions on a domain Ω, but nevertheless they are rather different objects. Their different characters should be reflected by any discretization procedure. Without specifying neither the discretization procedure in detail nor the boundary conditions we formulate a discrete stationary Schrödinger–Poisson problem and define a property (cf. (2.1) below) which guarantees that the discretized problem is also a variational problem with a boundedly Lipschitz continuous strongly monotone potential operator. These properties guarantee the discrete stationary Schrödinger-Poisson problem to be uniqely solvable and the convergence of the method of steepest gradient applied to the problem.

2. A discrete stationary Schrödinger–Poisson system

Let $M > 1$ be a fixed natural number corresponding to the number of knots of a grid for the domain Ω. As in the continuous case the equilibrium state of an electron system with a self-consistent potential is described by some statistics applied to the eigenvalues and eigenstates of the Hamiltonian $H = H_0 + V$ for a single electron. In our discrete case the space C^M with its usual scalar product is the Hilbert space. Thus the Hamiltonian is a $M \times M$ Hermite matrix $\mathbf{H}$. The matrix consists of a fixed Hermite part $\mathbf{H}_0$ and a Hermite part $\mathbf{V}$ due to the electrostatic potential of the electric charge of the whole system. This charge consists of a given positive charge density $0 \neq D \in R^M, D_j \geq 0$, and the unknown electron density N. The electrostatic potential V of the electric charge is self–consistently determined by a discrete analogon of the Poisson equation under homogeneous boundary conditions,

$$\mathbf{A}V = N - D,$$

where $\mathbf{A}$ is a real symmetric positive definite matrix. The Hamiltonian of the total system is

$$\mathbf{H} = \mathbf{H}(V) = \mathbf{H}_0 + \sum_{j=1}^{M} V_j \mathbf{H}_j = \mathbf{H}_0 + \mathbf{V}$$

with fixed Hermite matrices $\mathbf{H}_0, \mathbf{H}_1, ..., \mathbf{H}_M$. The operator $\mathbf{V}$ is the discretization of the multiplication operator $\psi \mapsto V\psi$ in $L_2(\Omega)$. In general, a discretization will not provide Hermite matrices $\mathbf{H}_1, ..., \mathbf{H}_M$, but we admit here only such discretizations which provide positive semidefinite Hermite matrices $\mathbf{H}_1, ..., \mathbf{H}_M$. We assume, moreover, that

$$\sum_{j=1}^{M} \mathbf{H}_j = \text{unit matrix } \mathbf{I}. \tag{2.1}$$

This assumption looks quite natural. In a first step the eigenvalue problem in $L_2(\Omega)$ may be discretized in such a way that the matrix formulation becomes

$$(\tilde{H}_0 + \sum_{j=1}^{M} V_j \tilde{H}_j)\psi = \epsilon \sum_{k=1}^{M} \tilde{H}_k \psi,$$

where the $\tilde{H}_j$ are symmetric positive semidefinite matrices, but their sum $\mathbf{J}$ is positive definite. Diagonalizing the scalar product $(\phi, \mathbf{J}\psi)$ by the transformation

$$\psi \mapsto \mathbf{J}^{1/2}\psi, \quad \tilde{H} \mapsto \mathbf{J}^{-1/2}\tilde{H}\mathbf{J}^{-1/2}$$

provides the property (2.1).
Let $\epsilon_1^V, ..., \epsilon_M^V$ be the eigenvalues of the operator $\mathbf{H} = \mathbf{H}(V)$ with an arbitrary $V \in R^M$ and let $(\psi_1^V, ..., \psi_M^V)$ be a corresponding frame of orthonormal eigenvectors. For the statistics we need a real function f like $\exp(-t)$ or $1/(1+\exp(t))$ as an energy distribution function. We consider a smooth nonnegative function f on the real line with the properties

(1) $f'(t) < 0 < f(t)$,
(2) $lim_{t \to +\infty} f(t) = 0$,
(3) $0 < d := \sum_{j=1}^{M} D_j < M \sup_t f(t)$.

Because of the last property of f the following definition of the Fermi level φ_D of the electron system makes sense.

Definition 2.1. The real-valued function φ_D on R^M which is implicitely defined by

$$\sum_l f[\epsilon_l^V - \varphi_D(V)] \;:=\; d$$

is called the **Fermi level** (with respect to f) of the quantum system with the Hamilton operator $\mathbf{H} = \mathbf{H}(V) = \mathbf{H}_0 + \sum_{j=1}^{M} V_j \mathbf{H}_j = \mathbf{H}_0 + \mathbf{V}$ and with the doping profile D. Following [11] the function defined on R^M by

$$F(V) \;:=\; \varphi_D(V) \sum_{m=1}^{M} f[\epsilon_m^V - \varphi_D(V)] \;-\; \sum_{l=1}^{M} \int_{\epsilon_l^V - \varphi_D(V)}^{\infty} f.$$

is called the **energy function** for the system.

Theorem 2.1. *The Fermi level and the energy function F are smooth functions on R^M. The gradient ∇F of F has the components*

$$\partial_j F(V) \;=\; \sum_{m=1}^{M} f[\epsilon_m^V - \varphi_D(V)](\psi_m^V, \mathbf{H}_j\psi_m^V) \;=:\; N_j(V)$$

$(j = 1, ..., M)$.

Proof. Let $U \in R^M$ be an arbitrary fixed vector. According to the theory of selfadjoint perturbations initiated by theorems of F. Rellich there is a complex open neighbourhood $G_M \subset C^M$ of U on which there are analytic functions $\Lambda_1, ..., \Lambda_M$ (some of them may be identical) and analytic frames $(\Psi_1, ..., \Psi_M)$ in C^M such that

$$\mathbf{H}(W)\Psi_m(W) = \Lambda_m(W)\Psi_m(W) \qquad (W \in G_M, m = 1, ..., M)$$

and

$$(\Psi_l(V), \Psi_m(V)) = \delta_{lm} \qquad (V \in G_M \cap R^M, 1 \leq l, m \leq M)$$

(cf. [14] chap. XII, problem 17). Thus the sets

$$\{\Lambda_1(V), ..., \Lambda_M(V)\} = \{\epsilon_1^V, ..., \epsilon_M^V\}$$

are the same. It follows from the implicite function theorem applied to $\Phi(V, Y) = \sum_m f[\Lambda_m(V) - Y]$ that the Fermi level φ_D is smooth on $G_M \cap R^M$. Then the function F is evidently smooth there. Straightforward differentiation provides

$$\nabla\varphi_D = \frac{\sum_m f_m' \nabla\Lambda_m}{\sum_l f_l'} \tag{2.2}$$

and

$$\nabla F = \nabla\varphi_D \sum_m f_m + \sum_l f_l \nabla[\Lambda_l - \varphi_D] = \sum_m f_m \nabla\Lambda_m \tag{2.3}$$

where $f_m = f[\Lambda_m(V) - \varphi_D(V)] = f[\epsilon_{k_m}^V - \varphi_D(V)]$. The identity

$$\partial_j\Lambda_m(U) = (\psi_m, \mathbf{H}_j\psi_m) \qquad (\psi_m = \Psi_m(U)) \tag{2.4}$$

is obtained by differentiating the identity

$$\Lambda_m(V)(\psi_m, \Psi_m(V)) = (\psi_m, \mathbf{H}(V)\Psi_m(V))$$

and by setting $V = U$. The identity

$$\sum_m f[\epsilon_m^U - \varphi_D(U)](\psi_m^U, \mathbf{H}_j\psi_m^U) = \sum_l f[\Lambda_l^U - \varphi_D(U)](\psi_l, \mathbf{H}_j\psi_l)$$

is proved elementarily regarding that there are unitary matrices $\mathbf{C}^V$ such that $\psi_l^V = \sum_m C_{lm}^V \Psi_m(V)$ with $C_{lm}^V = 0$ if $\epsilon_l^V \neq \Lambda_m(V)$. We have seen that φ_D and the function F are smooth on a neighbourhood of an arbitrary point $U \in R^M$, i.e. they are smooth functions. $\square$

We have assumed that the matrices $\mathbf{H}_j$ are positive semidefinite. Therefore the vector $N(V) = \nabla F(V)$ can be interpreted as a density. The property (2.1) guarantees that the definition of the Fermi level is equivalent to the charge neutrality of the system, indeed

$$\sum_j N_j = \sum_j \sum_m f_m(\psi_m^V, \mathbf{H}_j \psi_m^V) = \sum_m f_m(\psi_m^V, \sum_j \mathbf{H}_j \psi_m^V) = \sum_m f_m(\psi_m^V, \psi_m^V)$$

$$= \sum_m f_m = d.$$

The equality $N_j(V) = \sum_m f_m |\psi_{mj}^V|^2$ holds if and only if the operator $\mathbf{V}$ is just the diagonal matrix $V*$ corresponding to the vector V.

Definition 2.2. The **discrete stationary Schrödinger–Poisson problem** is to find a potential $V \in R^M$ which satisfies the vector equation $\mathbf{A}V = N(V) - D$.

Let us use the notation as in the proof of the preceding theorem, but let us assume, furthermore, that the eigenvalues $\lambda_m = \Lambda_m(U)$ are simple. We differentiate the identities

$$[\Lambda_l(V) - \lambda_m](\psi_m, \Psi_l(V)) = (\psi_m, (\mathbf{V} - \mathbf{U})\Psi_l(V)) \qquad (1 \leq l \neq m \leq M)$$

with respect to V_j and set $V = U$. As the result we get

$$(\psi_m, \partial_j \Psi_l(U)) = \frac{(\psi_m, \mathbf{H}_j \psi_l)}{\lambda_l - \lambda_m}. \tag{2.5}$$

Similarly one gets

$$\Re(\psi_m, \partial_j \Psi_m(U)) = 0 \qquad (m = 1, ..., M)$$

for the real part of the scalar products. In the following we use the summation convention with respect to the indices a and apply the differential operator $X_a \partial_a = X\nabla$ with respect to V. Thus

$$(X\nabla X)^2 \; F(V) \;=\; X\nabla \; [\sum_m f_m \; X\nabla\Lambda_m] \;=$$

$$\sum_m f'_m \; [X\nabla(\Lambda_m - \varphi_D)] \; X\nabla\Lambda_m \; + \sum_l f_l X\nabla \; (X\nabla\Lambda_l) =: S + T.$$

Substituting $\nabla\varphi_D$ in S by (2.2) and abbreviating $X\nabla\Lambda_m =: \omega_m$ we get

$$S = \sum_m f'_m \omega_m^2 - \sum_m f'_m \{\sum_l f'_l \omega_l \frac{\omega_m}{\sum_k f'_k}\}$$

i.e.

$$S \sum_k f'_k = \sum_l \sum_m f'_l f'_m (\omega_l^2 - \omega_l \omega_m) = \sum_l \sum_{m<l} f'_l f'_m (\omega_l - \omega_m)^2 \geq 0$$

or $S \leq 0$, since $\sum_k f'_k < 0$.

The summand T can be estimated by means of (2.4). Applying

$$X\nabla\ (X\nabla\Lambda_m) = X\nabla(\Psi_m(V), \mathbf{X}\Psi_m(V)) =$$
$$(X\nabla\Psi_m(V)\ ,\ \mathbf{X}\Psi_m(V)) + (\Psi_m(V)\ ,\ \mathbf{X}\ X\nabla\Psi_m(V)) =$$
$$= 2\Re(\ \mathbf{X}\Psi_m(V)\ ,\ X\nabla\Psi_m(V)\ ) = 2\Re(\ \sum_l \psi_l(\psi_l, \mathbf{X}\Psi_m(V))\ ,\ X\nabla\Psi_m(V)\ ) =$$
$$2\Re\{X_a(\psi_m, \mathbf{X}\Psi_m(V))(\psi_m, \partial_a\Psi_m(V)) + \sum_{l\neq m} X_a(\mathbf{X}\Psi_m(V), \psi_l)(\psi_l, \partial_a\Psi_m(V))\}$$
$$= 2\Re\sum_{l\neq m}\frac{(\mathbf{X}\psi_m, \psi_l)(\psi_l, \mathbf{X}\psi_m)}{\lambda_m - \lambda_l} = 2\sum_{l\neq m}\frac{\omega_{ml}}{\lambda_m - \lambda_l}$$

with $\omega_{ml} = |(\psi_l, \mathbf{X}\psi_m)|^2 = \omega_{lm}$, we get

$$T = 2\sum_m f_m \sum_{l\neq m}\frac{\omega_{ml}}{\lambda_m - \lambda_l} = 2\sum_m\sum_{l<m}\frac{f_m - f_l}{\lambda_m - \lambda_l}\omega_{ml} \leq 0,$$

since f decreases.
In the case that the eigenvalues of $\mathbf{H}(U)$ are simple, we have seen that

$$X_a X_b \partial_b \partial_a F(U) \leq 0 \qquad (X \in R^M).$$

The result does not really depend upon the simplicity of the eigenvalues, but the proof given just before makes use of the identities (2.5) the right-hand side of which may be an indefinite expression in the case of multiple eigenvalues. In the general case another proof works. It is based on Dunford's integral calculus for operators.

3. Application of Dunford's integral calculus

From now on we assume that the function $-\int_t^\infty f$ is the restriction onto the real line $R \subset C$ of a complex analytic function h on an open neighbourhood $G \subset C$ of R. Then f is the restriction onto R of the derivative h' of h. In this case the Fermi level and the energy function F are restrictions onto R^M of complex analytic functions $\tilde{\varphi_D}$ and $\tilde{F}$, respectively, defined on a complex open neighbourhood $\tilde{G}_M \subset C^M$ of $R^M \subset C^M$. Let $K_{00} \subset R^M$ be an arbitrary bounded set (in the proofs of local statements $K_{00} = \{U\}$ with an arbitrary $U \in R^M$). A properly chosen neighbourhood $G_M \subset \tilde{G}_M$ of K_{00} can be covered by a finite number J of open sets $G_M^\iota \subset C^M$ as in the proof of Theorem 2.1. If Λ_m^ι and Ψ_m^ι have the same meaning as in the proof of that theorem, then the closures

$$K_0^\iota = \mathrm{cl}\{\Lambda_m^\iota(V) :\ 1 \leq m \leq M,\ V \in G_M^\iota \cap R^M\}$$

and

$$K^\iota = \mathrm{cl}\{\lambda - \varphi_D(V) :\ \lambda \in K_0^\iota,\ V \in G_M^\iota \cap R^M\}$$

are compact sets in R. Let $\Gamma \subset G$ be a path which is the boundary of an open simply connected neighbourhood of $G_K \subset C$ of $K = \cup_{\iota=1}^J K^\iota$ such that Cauchy's integral formula is applicable. Then for any analytic function g on G_K, which is continuous on $\bar{G}_K = G_K \cup \Gamma$ there is an matrix-valued function

$$g[\mathbf{H}(V)] = \frac{1}{2\pi i}\int_\Gamma g(\lambda)[\lambda - \mathbf{H}(V)]^{-1} d\lambda =: \int g(\lambda)[\lambda - \mathbf{H}(V)]^{-1} d_\Gamma\lambda\ .$$

The values $g[\mathbf{H}(V)]$ do not depend on the special contour Γ which encloses the spectrum of $\mathbf{H}(V)$. The function depends smoothly on $V \in G_M \cap R^M$. Indeed, since

$$
\begin{aligned}
g[\mathbf{H}(V+tX)] - g[\mathbf{H}(V)] &= g(\mathbf{H}+t\mathbf{X}) - g(\mathbf{H}) \\
&= \int g(\lambda)\left[(\lambda - \mathbf{H} - t\mathbf{X})^{-1} - (\lambda - \mathbf{H})^{-1}\right] d_\Gamma\lambda \\
&= \int g(\lambda)\left[(\lambda - \mathbf{H} - t\mathbf{X})^{-1} t\mathbf{X}(\lambda - \mathbf{H})^{-1}\right] d_\Gamma\lambda\ ,
\end{aligned}
$$

the identities

$$
X\nabla g[\mathbf{H}(V)] = \int g(\lambda)\left[(\lambda - \mathbf{H})^{-1}\mathbf{X}(\lambda - \mathbf{H})^{-1}\right] d_\Gamma\lambda, \tag{3.1}
$$

$$
(X\nabla X)^2 g[\mathbf{H}(V)] = 2\int g(\lambda)\left\{(\lambda - \mathbf{H})^{-1}[\mathbf{X}(\lambda - \mathbf{H})^{-1}]^2\right\} d_\Gamma\lambda \tag{3.2}
$$

hold.
The trace of a matrix $\mathbf{A}$ is $\mathrm{Tr}(\mathbf{A}) = \sum_{l=1}^{M}(e_l, \mathbf{A}e_l)$ for any orthonormal basis $(e_1, ..., e_M)$ in C^M. Choosing,in particular, $e_l = \Psi_l(V)$ $(l = 1, ..., M)$ for the matrix

$$
g[\mathbf{H}(V)] = \sum_{m=1}^{M} g[\Lambda_m(V)]\Psi_m(V) \otimes \Psi_m(V)^*
$$

with a real $V \in G_M \cap R^M$ we get

$$
\mathrm{Tr}\{g[\mathbf{H}(V)]\} = \sum_{m=1}^{M} g[\Lambda_m(V)]. \tag{3.3}
$$

This identity provides a connection between the formulas of the preceding section and the formulas which will be derived below.
Thus the Fermi level and the energy function can be redefined by

$$
d = \mathrm{Tr}\{\ h'[\mathbf{H}(V) - \varphi_D(V)]\ \}, \tag{3.4}
$$

$$
F(V) = \varphi_D(V)\ \mathrm{Tr}\{h'[\mathbf{H}(V) - \varphi_D(V)]\} + \mathrm{Tr}\{h[\mathbf{H}(V) - \varphi_D(V)]\}. \tag{3.5}
$$

Furthermore, we get

$$
\begin{aligned}
&X\nabla\ \mathrm{Tr}\{g[\mathbf{H}(V)]\} = \mathrm{Tr}\{X\nabla\{g[\mathbf{H}(V)]\}\} \\
&= \int g(\lambda)\mathrm{Tr}[(\lambda - \mathbf{H})^{-1}\mathbf{X}(\lambda - \mathbf{H})^{-1}]\ d_\Gamma\lambda = \int g(\lambda)\mathrm{Tr}[(\lambda - \mathbf{H})^{-2}\mathbf{X}]\ d_\Gamma\lambda \\
&= \mathrm{Tr}\left[\int g(\lambda)(\lambda - \mathbf{H})^{-2}\ d_\Gamma\lambda\ \mathbf{X}\right] = \mathrm{Tr}[g'(\mathbf{H})\mathbf{X}].
\end{aligned}
$$

with regard to (3.1) and the idendity $\mathrm{Tr}(\mathbf{AB}) = \mathrm{Tr}(\mathbf{BA})$, i.e. the identity

$$
X\nabla\mathrm{Tr}\{g[\mathbf{H}(V)]\} = \mathrm{Tr}\{X\nabla\{g[\mathbf{H}(V)]\}\} = \mathrm{Tr}\{g'[\mathbf{H}(V)]\ \mathbf{X}\} \tag{3.6}
$$

holds.
If a family of analytic functions $g(., Y)$ on G_K depends smoothly on a real parameter Y, then the matrix family $g[\mathbf{H}(V), Y]$ depends smoothly on Y, too. In our case

$$
g(\lambda, Y) = Yh'(\lambda - Y) + h(\lambda - Y) \quad \text{and} \quad Y = \varphi_D(V)\ .
$$

We mention the identity

$$\partial_Y \mathrm{Tr}[h(\mathbf{H}-Y)] = -\mathrm{Tr}[h'(\mathbf{H}-Y)]. \tag{3.7}$$

Regarding the definition of the Fermi level and the listed formulas we get

$$X\nabla F(V) = [X\nabla\varphi_D(V)]\mathrm{Tr}\{h'[\mathbf{H}(V)-\varphi_D(V)]\} + \mathrm{Tr}\{X\nabla\{h[\mathbf{H}(V)-\varphi_D(V)]\}\}$$
$$= \mathrm{Tr}\{h'[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X}\} = \sum X_j\,\mathrm{Tr}\{h'[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{H}_j\} = \sum_j X_j N_j(V).$$

4. The variational formulation of the nonlinear vector equation

Theorem 4.1. *The matrix $d^2F(V)$ of the partial second-order derivatives is negative semidefinite for any $V \in R^M$.*

Proof. Using the last identity of the preceding section we start with

$$(X\nabla)^2F(V) = \mathrm{Tr}\{X\nabla\{h'[\mathbf{H}(V)-\varphi_D(V)]\}\,\mathbf{X}\}.$$

Applying (3.6) and (3.7) we get

$$(X\nabla)^2F(V) = \mathrm{Tr}\left\{h"[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X}^2 - [X\nabla\varphi_D(V)]\,h"[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X}\right\}.$$

Instead of rewriting (2.2) by means of (2.4) the expression $X\nabla\varphi_D(V)$ is obtained by differentiating (3.4).

$$0 = \mathrm{Tr}\{X\nabla\{h'[\mathbf{H}(V)-\varphi_D(V)]\}\}$$
$$= \mathrm{Tr}\{\,h"[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X} - [X\nabla\varphi_D(V)]\,h"[\mathbf{H}(V)-\varphi_D(V)]\,\}.$$

According to the assumptions concerning f the trace

$$\mathrm{Tr}\{h"[\mathbf{H}(V)-\varphi_D(V)]\} < 0$$

does not vanish. Thus

$$X\nabla\varphi_D(V) = \frac{\mathrm{Tr}\{\,h"[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X}\,\}}{\mathrm{Tr}\{h"[\mathbf{H}(V)-\varphi_D(V)]\}} \tag{4.1}$$

and thus

$$(X\nabla)^2F(V) = \mathrm{Tr}\{\,h"[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X}^2\,\} - \frac{(\mathrm{Tr}\{\,h"[\mathbf{H}(V)-\varphi_D(V)]\,\mathbf{X}\,\})^2}{\mathrm{Tr}\{h"[\mathbf{H}(V)-\varphi_D(V)]\}}.$$

The operator $h"[\mathbf{H}(V)-\varphi_D(V)]$ is a diagonal matrix $\mathbf{B} = B*$ with respect to the orthonormal basis $(\Psi_1(V), ..., \Psi_M(V))$. Their diagonal elements are $B_j = f'[\Lambda_j(V)-\varphi_D(V)] \leq 0$. The symmetric operators $\mathbf{X}$ are Hermite matrices $\mathbf{Y}$ with respect to this basis. Thus the inequality

$$\mathrm{Tr}\{h"[\mathbf{H}(V)-\varphi_D(V)]\}\,(X\nabla)^2F(V) = \mathrm{Tr}(\mathbf{B})\,\mathrm{Tr}(\mathbf{YBY}) - [\mathrm{Tr}(\mathbf{BY})]^2$$
$$= \sum_k\sum_{j<k} B_jB_k(Y_{kk}-Y_{jj})^2 + \sum_j\sum_k B_jB_k\sum_{l\neq k}|Y_{kl}|^2 \geq 0$$

is checked quite elementary, i.e.

$$(X\nabla)^2F(V) \leq 0$$

for any real X, $V \in R^M$, because $\mathrm{Tr}\{h"[\mathbf{H}(V) - \varphi_D(V)]\} = \sum_j B_j < 0$. In other words, the set $\hat{F} := \{(V,Y) \in R^M \times R : Y \le F(V)\}$ is convex. $\square$

As an easy consequence of theorems 2.1 and 4.1 we get the variational formulation of the discrete stationary Schrödinger–Poisson problem together with its unique solvability.

Theorem 4.2. *A vector $U \in R^M$ is a solution of the nonlinear problem $\mathbf{A}V = N(V) - D$ if and only if the vector U minimizes the strictly convex functional*

$$G(V) := \frac{1}{2}(V, \mathbf{A}V) + (D,V) - F(V)\ .$$

5. A Remark on the Choice of M

For a given Schrödinger-Poisson equation the influence of eigenstates with higher and higher energy levels of the associated eigenvalue problem becomes smaller and smaller. If the problem is to be solved, only a finite number L of lowest eigenstates can be regarded at all. These eigenstates can be calculated only approximately on a finite grid of $M \ge L$ knots, and $M > L$ is reasonable to be expected. This reflection suggested, on the other hand, a modification of the discrete stationary Schrödinger- Poisson problem.

Let us assume that there are an integer L between 1 and M and a function Λ^L on R^M such that

(1) $d < L \sup_t f(t)$,

(2) for any $V \in R^M$ the set

$$I_V^L := \{m : 1 \le m \le M,\ \epsilon_m^V \le \Lambda^L(V)\}$$

consists of exactly L indices.

Then we define a Fermi level φ_D^L and an energy function F^L by

$$d =: \sum_{m \in I_V^L} f[\epsilon_m^V - \varphi_D^L(V)]$$

and

$$F^L(V) := \varphi_D^L(V) \sum_{l \in I_V^L} f[\epsilon_l^V - \varphi_D^L(V)] - \sum_{m \in I_V^L} \int_{\epsilon_m^V - \varphi_D^L(V)}^{\infty} f,$$

respectively. The analogues of theorems 2.1, 4.1, and 4.2 hold for φ_D^L and F^L, too. Indeed, let $U \in G_M \subset R^M$, $\Lambda_1, ..., \Lambda_M$, $\Psi_1, ..., \Psi_M$ have the same meaning as in the proof of theorem 2.1. Let denote

$$J_U^L := \{l : 1 \le l \le M,\ \Lambda_l(U) \le \Lambda^L(U)\}$$

and CJ_U^L the complement of J_U^L in $\{1, ..., M\}$. Then there is a complex open neighbourhood of U, without any restriction of generality G_M itself, such that

$$\max_{l \in J_U^L} \Lambda_l(V) < \min_{m \in CJ_U^L} \Lambda_m(V) \qquad (V \in G_M \cap R^M).$$

The existence of such a 'gap' in the spectrum of the 'discrete' electron is the consequence of and the reason for the assumption made above. Unfortunately, we do not know, how restrictive the assumption is. The smoothness of the Fermi level φ_D^L in $G_M \cap R^M$ follows again from the implicite function theorem applied to the function

$$\Phi_L(V,Y) \;=\; \sum_{m\in J_U^L} f[\Lambda_m(V) - Y].$$

Dunford's integral calculus claims some more attention than above, as the operators

$$g_L[\mathbf{H}(V)] \;=\; \int g(\lambda)[\lambda - \mathbf{H}(V)]^{-1}\, d_{\Gamma_U^L}$$

are defined with a closed curve Γ_U^L which encloses only the poles $\Lambda_l(V),\ l \in J_U^L$, of $[\lambda - \mathbf{H}(V)]^{-1}$, but not $\Lambda_m(V),\ m \in CJ_U^L$.
The Fermi levels were defined by

$$\sum_{J_U^L} f_l^L \;:=\; \sum_{J_U^L} f[\Lambda_l(V) - \varphi_D^L(V)] \;=\; d \;=\; \sum_{J_U^L} f_l \;+\; \sum_{CJ_U^L} f_m \;\geq\; \sum_{J_U^L} f_l,$$

where f_l denotes $f[\Lambda_l(V) - \varphi_D(V)]$. Therefore there is at least one $n \in J_U^L$ such that $f_n^L \;\geq\; f_n$. Since f is a monotonously decreasing function, the inequality

$$\varphi_D^L(V) \geq \varphi_D(V) \tag{5.1}$$

holds. Thus we have $f_l^L \geq f_l$ for all $l \in J_U^L$ and

$$\sum_{J_U^L}(f_l^L - f_l) \;=\; \sum_{CJ_U^L} f_m \;=:\; \eta^L(V). \tag{5.2}$$

Furthermore, we get $F^L \geq F$ because of

$$\begin{aligned} F^L(V) - F(V) = d[\varphi_D^L(V) - \varphi_D(V)] \;&-\; \sum_{J_U^L}\Big(\int_{\Lambda_l-\varphi_D^L} f - \int_{\Lambda_l-\varphi_D} f\Big) \;+\; \sum_{CJ_U^L}\int_{\Lambda_m-\varphi_D^L} f \\ \geq\; d[\varphi_D^L(V) - \varphi_D(V)] \;&-\; \sum_{J_U^L}\int_{\Lambda_l-\varphi_D^L}^{\Lambda_l-\varphi_D} f \\ &\geq\; [\varphi_D^L(V) - \varphi_D(V)]\,(d - \sum_{J_U^L} f_l^L) \;=\; 0. \end{aligned}$$

The function η^L attains positive values $\leq d$. As the following theorem shows, integers $L < M$ are of interest for which $\eta^L(V) << d$.

Theorem 5.1. *Let α denote the 'ellipticity constant' of the matrix $\mathbf{A}$. Then the estimate*

$$\begin{aligned} \alpha|\hat{V} - V^L|_\infty \;&\leq\; \min\Big[\; |N(\hat{V}) - N^L(\hat{V})|_1 \;,\; |N(V^L) - N^L(V^L)|_1 \;\Big] \\ &\leq\; 2\min\Big[\eta^L(\hat{V}), \eta^L(V^L)\Big] \end{aligned}$$

holds for the difference of the vectors $\hat{V}$ and V^L which minimize the functions G or $G^L(V) := \frac{1}{2}(V,\mathbf{A}V) + (D,V) - F^L(V)$, respectively.

Proof. The difference of the identities

$$\begin{aligned}(W, \mathbf{A}\hat{V}) &= (W, N(\hat{V}) - D) \qquad (W \in R^M),\\ (W, \mathbf{A}V^L) &= (W, N^L(V^L) - D) \qquad (W \in R^M)\end{aligned}$$

for $W = \hat{V} - V^L$ gives

$$\begin{aligned}\alpha|\hat{V} - V^L|_\infty^2 &\leq (\hat{V} - V^L, \mathbf{A}(\hat{V} - V^L)) = (\hat{V} - V^L, N(\hat{V}) - N^L(V^L))\\ &= (\hat{V} - V^L, N^L(\hat{V}) - N^L(V^L)) + (\hat{V} - V^L, N(\hat{V}) - N^L(\hat{V}))\\ &\leq (\hat{V} - V^L, N(\hat{V}) - N^L(\hat{V})) \leq |\hat{V} - V^L|_\infty \, |N(\hat{V}) - N^L(\hat{V})|_1,\end{aligned}$$

since the operator N^L is monotone. An analogous estimate with the factor $|N(V^L) - N^L(V^L)|_1$ on the right-hand side is obtained, because N is also monotone. Furthermore,

$$\begin{aligned}|N(V) - N^L(V)|_1 &= \sum_j |N_j(V) - N_j^L(V)|\\ &= \sum_j \Big| \sum_{m=1}^{M} f_m(\Psi_m(V), \mathbf{H}_j\Psi_m(V)) - \sum_{J_U^L} f_l^L(\Psi_l(V), \mathbf{H}_j\Psi_l(V))\Big|\\ &= \sum_j \sum_{CJ_U^L} f_m(\Psi_m(V), \mathbf{H}_j\Psi_m(V)) + \sum_j \sum_{J_U^L} (f_l - f_l^L)(\Psi_l(V), \mathbf{H}_j\Psi_l(V))\\ &= \sum_{CJ_U^L} f_m + \sum_{J_U^L} (f_l - f_l^L) \leq 2\eta_L(V).\end{aligned}$$

□

The theorem gives some rough hints of the proper choice of M. The number M should be large enough for a given problem, if there is an $L \approx M/2$ for which $\eta^L(V^L) << d$.

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