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The Birman–Solomyak theorem revisited: A novel elementary proof, generalisation, and applications

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Abstract

We provide a new short proof for the Birman–Solomyak theorem for Hilbert–Schmidt operators and give an application to a Schrödinger–Poisson system.

1 Introduction

About sixty years ago, Birman and Solomyak developed their calculus of double operator spectral integrals, see [BS1] [BS2] [BS3] and derived, among other results, estimates of the form

$$\|f(A) - f(B)\|_{\mathcal{S}_p} \leq L(f)\, \|A - B\|_{\mathcal{S}_p}, \tag{1.1}$$

where A, B are bounded, self-adjoint operators, $f\colon \mathbb{R} \to \mathbb{R}$ is a function from an adequate class, $L(f) < \infty$ is a suitable constant depending only on f, and $\|\cdot\|_{\mathcal{S}_p}$ is a Schatten norm. A directly accessible case of (1.1) is $p = 2$, where the Lipschitz property of f is sufficient for (1.1), with $L(f)$ being the Lipschitz constant of f. Birman and Solomyak remarked in [BS4] page 156 that, in spite of this simple characterisation, an elementary proof of (1.1) for $p = 2$ was lacking for a long time, and it was eventually given by Gesztesy, Pushnitski and Simon more than forty years later in [GPS]. Their approach is based on a classical theorem of Löwner [Löw] for finite-dimensional operators complemented by suitable limit arguments. We became interested in (1.1) when one of us applied it in [KR1] [KR2] for the derivation of estimates for particle density operators in the Kohn–Sham system.

The first aim of this paper is to give an elementary proof of (1.1) for $p = 2$, which is quite different from the one in [GPS] and to generalise (1.1) for the case $p = 2$ to arbitrary *unbounded* self-adjoint operators, provided $f\colon \mathbb{R} \to \mathbb{R}$ is (globally) Lipschitz continuous. More precisely, we prove the following theorem, in which, for a given Hilbert space $\mathcal{H}$, we denote by $\mathcal{L}_{\mathrm{HS}}(\mathcal{H})$ the Hilbert space of all Hilbert–Schmidt operators and Hilbert–Schmidt norm $\|\cdot\|_{\mathrm{HS}}$.

Theorem 1.1. *Let A, B be two self-adjoint operators in a Hilbert space H. Let $C \in \mathcal{L}_{\mathrm{HS}}(H)$ and suppose that $A = B + C$. Let $f\colon \mathbb{R} \to \mathbb{R}$ be a Lipschitz continuous function with Lipschitz constant L. Then $D(A) = D(B) \subset D(f(A)) = D(f(B))$ and the operator $f(A) - f(B)$ extends to a Hilbert–Schmidt operator, by abuse of notation still denoted by $f(A) - f(B)$, such that*

$$\|f(A) - f(B)\|_{\mathrm{HS}} \leq L\, \|C\|_{\mathrm{HS}}. \tag{1.2}$$

In our proof of Theorem 1.1 we first assume that f is bounded and that A and B have pure point spectrum, which includes all compact operators and those with compact resolvent. In contrast to [GPS] our proof only requires Parseval's identity. Having this at hand, we employ an argument quite similar to one in [GPS] to carry this over to the class of all self-adjoint operators A, B, still with the Hilbert–Schmidt

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condition. Finally, an approximation argument allows us to eliminate the boundedness assumption for f. While our proof of (1.1) in case that $p = 2$ does not generalise to other Schatten classes with $p \neq 2$, we note that Peller [Pel] succeeded in proving (1.1) for $p \neq 2$ by using double and triple sums instead of the calculus of double spectral integrals.

Secondly, we deduce from (1.2) estimates of the form

$$\|f(A) - f(B)\|_{\mathrm{HS}} \leq K \, \|(A + \lambda)^{-1} - (B + \lambda)^{-1}\|_{\mathrm{HS}}, \tag{1.3}$$

where $K > 0$ depends on the Lipschitz constant of f and λ. For smooth functions f with a certain decay the estimate (1.3) is also in [GN] (3.5) for general Schatten classes. The proof in [GN] involves the Helffer–Sjöstrand calculus, which is much more complicated. The importance of (1.3) lies in the fact that, e.g., for Schrödinger operators, the difference of $A = -\operatorname{div}\big(\mathfrak{m}^{-1}\nabla\big) + U$ and $B = -\operatorname{div}\big(\mathfrak{m}^{-1}\nabla\big) + V$ is usually not a Hilbert–Schmidt operator, but the difference of their resolvents often is. Note that for the validity of (1.3) only Lipschitz continuity of f is required. In particular, f does not need to be smooth, nor compactly supported and no almost analytic extension of f is required. We further remark that an estimate similar to (1.3) was derived and used in [KR1] and [KR2] for the estimation of density matrices with respect to Schrödinger potentials.

The third part of the paper is devoted to an application of the Birman–Solomyak theorem in density functional theory, namely, in the investigation of the Schrödinger–Poisson system. The connection to the Birman–Solomyak theorem is the following. Let $\Omega \subset \mathbb{R}^d$, with $d \in \{1, 2, 3\}$, be a bounded Lipschitz domain and $f \colon \mathbb{R} \to (0, \infty)$ a strictly decreasing differentiable function with suitable asymptotics at ∞. Let $H = -\operatorname{div}\big(\mathfrak{m}^{-1}\nabla\big)$ be the unperturbed Schrödinger operator with mixed boundary conditions on $\partial\Omega$. If $U \in L_2(\Omega, \mathbb{R})$, then the spectrum of the Schrödinger operator $H + U$ on $L_2(\Omega)$ is purely discrete with sufficiently rapidly growing eigenvalues, hence for all $\mu \in \mathbb{R}$ the operator

$$f(H + U - \mu)$$

defines a density matrix, that is a positive trace-class operator, and the diagonal of its Schwartz kernel defines a particle density $\mathcal{N}(U) \in L_2(\Omega, \mathbb{R})$. More precisely, viewing a bounded function W as a multiplication operator, one can show that the map

$$W \mapsto \operatorname{tr}\big(f(H + U - \mu)\, W\big)$$

extends to a continuous linear functional on $L_2(\Omega)$, which can be represented by a function $\mathcal{N}(U) \in L_2(\Omega)$. In physics, the number $\mu \in \mathbb{R}$ is a Lagrange multiplier called the Fermi level. It ensures the normalisation condition $\operatorname{tr}\big(f(H + U - \mu)\big) = N$, where $N > 0$ is the particle number. In many applications, $U = V_0 + V$ is a small perturbation of a fixed reference potential $V_0 \in L_2(\Omega)$. Since the Schrödinger–Poisson system can be written as one single equation (see [Nie])

$$-\nabla \cdot \varepsilon \nabla V - \mathcal{N}(V_0 + V) = q, \tag{1.4}$$

one is interested in the functional analytic properties of the map $U \mapsto \mathcal{N}(U)$ from $L_2(\Omega)$ into $L_2(\Omega)$ and from $W^{1,2}(\Omega)$ into $W^{-1,2}(\Omega)$, see also [WPH] Subsection 3.5. In [Nie] it was proved that the operator from $W^{1,2}(\Omega)$ into $W^{-1,2}(\Omega)$ is antimonotone and locally Lipschitz continuous, so that the standard monotone theory with the Browder-Minty theorem applies. Unfortunately, the proofs in [Nie] are technically involved. We will use the Birman–Solomyak theorem to prove that $U \mapsto \mathcal{N}(U)$ is locally Lipschitz continuous from $L_2(\Omega)$ into $L_2(\Omega)$. In [KNR], however, the monotonicity of $U \mapsto \mathcal{N}(U)$ from $L_2(\Omega)$ into $L_2(\Omega)$ and from $W^{1,2}(\Omega)$ into $W^{-1,2}(\Omega)$ was established by an abstract operator-theoretic principle, without using specific properties of the concrete Schrödinger operators which are involved. Moreover, the proof in [KNR] is fairly simple.

Concerning the continuity properties, in [KR1] and [KR2] local Lipschitz continuity of the map $U \mapsto \mathcal{N}(U)$ from $L_2(\Omega)$ into $L_2(\Omega)$ was established, which implies, trivially, the local Lipschitz continuity from $W^{1,2}(\Omega)$ into $W^{-1,2}(\Omega)$. These two properties, (anti)monotonicity and local Lipschitz continuity, are the key ingredients for an adequate investigation of the Schrödinger–Poisson system (1.4). Since the latter is a fundamental model in modern physics (see [POM] for a recent overview), we recall the essentials of the analysis for this system. This includes both a derivation of the local Lipschitz continuity for the particle density operator and a description of the foundation of a numerical procedure, which is standard nowadays, and rests on a functional-analytic based contraction principle.

As already indicated, several ideas of this paper are already present in the quoted foregoing papers, frequently with complicated proofs. It is, however, our intention to present an entirely self-contained text on the Schrödinger–Poisson system, now based on elementary proofs of the crucial properties of the particle density operator and readable also for theoretical physicists. Essentially new in this paper is a deeper analysis of the Schrödinger operators. In particular it is proved that $H + V$ makes sense also as operator sum, and not only via forms. Moreover, a deeper analysis shows here that the resolvents of the operators $(H + U)$ map $L_2(\Omega)$ into $L_\infty(\Omega)$, and the corresponding norms are bounded, uniformly on L_2-bounded sets of potentials U. Moreover, in Theorem 5.1 we prove that the solution of the Schrödinger–Poisson system as function of the reference potential V_0 and the right hand side q also is locally Lipschitz. This is the key tool for the treatment of the Kohn–Sham system, see [KR1] [KR2]. We refer to [WPH] Section 3.5 for the numerics of the Kohn–Sham system.

The paper is organised as follows. In Section 2 we prove Theorem 1.1. In Section 3 we prove (1.3) on resolvents. We provide in Section 4 an abstract theorem to construct a solution for a strongly monotone operator via the Banach contraction theorem. In Theorem 5.1 we give a rigorous statement and proof of the Schrödinger–Poisson system (1.4) and show that the solution is (locally) Lipschitz as function of the data.

2 The elementary proof

If $(X, \mathcal{A}, \mu)$ is a measure space, then we say that $(X, \mathcal{A}, \mu)$ is a **locally finite** if for all $E \in \mathcal{A}$ with $\mu(E) = \infty$ there exists an $F \in \mathcal{A}$ such that $F \subset E$ and $0 < \mu(F) < \infty$. If A is an operator in a Hilbert space $\mathcal{H}$, then we provide $D(A)$ with the graph norm given by $\|u\|_{D(A)}^2 = \|Au\|_{\mathcal{H}}^2 + \|u\|_{\mathcal{H}}^2$.

We need some lemmas.

Lemma 2.1. *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and $f : \mathbb{R} \to \mathbb{R}$ a Lipschitz continuous function. Then one has the following.*

(a) $D(A) \subset D(f(A))$.

(b) $D(A)$ *is a core for* $f(A)$.

(c) *For all $n \in \mathbb{N}$ define $\chi_n : \mathbb{R} \to \mathbb{R}$ by $\chi_n = (-n) \vee x \wedge n$. Then $\lim_{n\to\infty}(\chi_n \circ f)(A)u = f(A)u$ for all $u \in D(f(A))$.*

Proof. Using the spectral theorem we may assume that $\mathcal{H} = L_2(X, \mathcal{A}, \mu)$ and A is the multiplication operator with a measurable function $h : X \to \mathbb{R}$, where $(X, \mathcal{A}, \mu)$ is a locally finite measure space. Since f is Lipschitz continuous, there are $L, b > 0$ such that $|f(x)| \le L\,|x| + b$ for all $x \in \mathbb{R}$. Now $f(A)$ is the multiplication operator with the function $f \circ h$.

'(a)'. Let $u \in D(A)$. Then $\int |h\,u|^2 < \infty$ and $\int |u|^2 < \infty$. Hence

$$\int |(f \circ h) \cdot u|^2 \leq \int |L\,|h| + b|^2\,|u|^2 \leq 2L^2 \int |h\,u|^2 + 2b^2 \int |u|^2 < \infty.$$

Therefore $u \in D(f(A))$.

'(b)'. Let $u \in D(f(A))$. If $n \in \mathbb{N}$, then $u\,\mathbb{1}_{[|h| \leq n]} \in D(A)$. Moreover,

$$\lim_{n\to\infty} \int |(f \circ h)\,u\,\mathbb{1}_{[|h|\leq n]}|^2 = \int |(f \circ h)\,u|^2$$

by the monotone convergence theorem. So

$$\lim_{n\to\infty} \|A(u - u\,\mathbb{1}_{[|h|\leq n]})\|_{\mathcal{H}}^2 = \lim_{n\to\infty} \int \Big(|(f \circ h)\,u|^2 - \int |(f \circ h)\,u\,\mathbb{1}_{[|h|\leq n]}|^2 \Big) = 0.$$

Similarly $\lim_{n\to\infty} \|u - u\,\mathbb{1}_{[|h|\leq n]}\|_{\mathcal{H}}^2 = 0$ and $\lim u\,\mathbb{1}_{[|h|\leq n]} = u$ in $D(A)$. Hence $D(A)$ is a core for $f(A)$.

'(c)'. If $n \in \mathbb{N}$ and $u \in D(f(A))$, then $|(\chi_n \circ f \circ h) \cdot u|^2 \leq |(f \circ h) \cdot u|^2$ and also $\lim_{n\to\infty} (\chi_n \circ f \circ h) \cdot u = (f \circ h) \cdot u$. Then the statement follows from the Lebesgue dominated convergence theorem. □

The next two lemmas are trivial.

Lemma 2.2. *Let A, B be operators in a Hilbert space $\mathcal{H}$ and $T \in \mathcal{L}(\mathcal{H})$. Let D be a subspace of $\mathcal{H}$. Suppose that D is a core for B, the operator A is closed and $Au = Bu + Tu$ for all $u \in D$. Then $D(B) \subset D(A)$ and $Au = Bu + Tu$ for all $u \in D(B)$.*

Proof. Let $u \in D(B)$. Then there exists a sequence $(u_n)_{n\in\mathbb{N}}$ in D such that $\lim u_n = u$ in $D(B)$. Now $\lim Au_n = \lim(Bu_n + Tu_n) = Bu + Tu$. Since A is closed, it follows that $u \in D(A)$ and $Au = Bu + Tu$. □

Lemma 2.3. *Let T be a densely defined symmetric operator in a Hilbert space $\mathcal{H}$. Let $(u_\alpha)_{\alpha\in I}$ be an orthonormal basis in $\mathcal{H}$. Suppose that $u_\alpha \in D(T)$ and $\sum_{\alpha\in I} \|Tu_\alpha\|_{\mathcal{H}}^2 < \infty$. Then T extends to a bounded operator on $\mathcal{H}$.*

Proof. Let $u \in D(T)$. Then

$$\|Tu\|_{\mathcal{H}}^2 = \sum_{\alpha\in I} |(Tu, u_\alpha)|^2 = \sum_{\alpha\in I} |(u, Tu_\alpha)|^2 \leq \sum_{\alpha\in I} \|u\|_{\mathcal{H}}^2\,\|Tu_\alpha\|_{\mathcal{H}}^2 = \|u\|_{\mathcal{H}}^2 \sum_{\alpha\in I} \|Tu_\alpha\|_{\mathcal{H}}^2$$

and the lemma follows. □

Now we prove Theorem 1.1 in the special case that A and B have a pure point spectrum. The proof is very elementary. For simplicity we assume that f is bounded.

Proposition 2.4. *Adopt the assumptions and notation of Theorem 1.1. Suppose in addition that A and B both have a pure point spectrum and that the function f is bounded. Then $f(A) - f(B)$ is a Hilbert–Schmidt operator and*

$$\|f(A) - f(B)\|_{\mathrm{HS}} \leq L\,\|C\|_{\mathrm{HS}}.$$

Proof. Since A has a pure point spectrum there exists an orthonormal basis $(u_\alpha)_{\alpha\in I}$ for $\mathcal{H}$ and for all $\alpha \in I$ there exists a $\lambda_\alpha \in \mathbb{R}$ such that $Au_\alpha = \lambda_\alpha\, u_\alpha$. Similarly for B there exists an orthonormal basis $(v_\alpha)_{\alpha\in I}$ for $\mathcal{H}$ and for all $\alpha \in I$ there exists a $\mu_\alpha \in \mathbb{R}$ such that $Bv_\alpha = \mu_\alpha\, v_\alpha$.

If $\alpha, \beta \in I$, then

$$\begin{aligned}((f(A) - f(B))u_\alpha, v_\beta)_{\mathcal{H}} &= (f(A)u_\alpha, v_\beta)_{\mathcal{H}} - (u_\alpha, f(B)v_\beta)_{\mathcal{H}} \\ &= (f(\lambda_\alpha)\, u_\alpha, v_\beta)_{\mathcal{H}} - (u_\alpha, f(\mu_\beta)\, v_\beta)_{\mathcal{H}} = (f(\lambda_\alpha) - f(\mu_\beta))\,(u_\alpha, v_\beta)_{\mathcal{H}}.\end{aligned}$$

Now let $\alpha \in I$. Then Parseval's identity gives

$$\begin{aligned}\|(f(A) - f(B))u_\alpha\|_{\mathcal{H}}^2 &= \sum_{\beta\in I} |((f(A) - f(B))u_\alpha, v_\beta)_{\mathcal{H}}|^2 = \sum_{\beta\in I} |f(\lambda_\alpha) - f(\mu_\beta)|^2\, |(u_\alpha, v_\beta)_{\mathcal{H}}|^2 \\ &\leq \sum_{\beta\in I} L^2\, |\lambda_\alpha - \mu_\beta|^2\, |(u_\alpha, v_\beta)_{\mathcal{H}}|^2 = L^2\, \|(A - B)u_\alpha\|_{\mathcal{H}}^2 = L^2\, \|Cu_\alpha\|_{\mathcal{H}}^2.\end{aligned}$$

Hence

$$\|f(A) - f(B)\|_{\mathrm{HS}}^2 = \sum_{\alpha\in I} \|(f(A) - f(B))u_\alpha\|_{\mathcal{H}}^2 \leq \sum_{\alpha\in I} L^2\, \|Cu_\alpha\|_{\mathcal{H}}^2 = L^2\, \|C\|_{\mathrm{HS}}^2 < \infty$$

and the proposition follows. □

We now drop the assumption that A and B have a pure point spectrum, but add the assumption that $\mathcal{H}$ is separable. The proof is a modification of the proof of [GPS] Theorem 4.1.

Proposition 2.5. *Adopt the assumptions and notation of Theorem* 1.1*. Suppose in addition that the function f is bounded and the Hilbert space $\mathcal{H}$ is separable. Then $f(A) - f(B)$ is a Hilbert–Schmidt operator and*

$$\|f(A) - f(B)\|_{\mathrm{HS}} \leq L\, \|C\|_{\mathrm{HS}}.$$

Proof. By Proposition 2.4 we my assume that $\mathcal{H}$ is infinite dimensional. Since $\mathcal{H}$ is separable and A is self-adjoint there exists an orthonormal basis $(e_k)_{k\in\mathbb{N}}$ for $\mathcal{H}$ with $e_k \in D(A)$ for all $k \in \mathbb{N}$. For all $n \in \mathbb{N}$ let P_n be the orthogonal projection of $\mathcal{H}$ onto $\mathrm{span}\{e_1, \ldots, e_n\}$, set $A_n = P_n\, A\, P_n$ and $B_n = P_n\, B\, P_n$. Now $\lim_{n\to\infty} A_n = A$ in the strong resolvent sense. Therefore $\lim_{n\to\infty} f(A_n) = f(A)$ strongly in $\mathcal{H}$ by [RS] Theorem VIII.20, where we use that f is bounded. In particular, $\lim_{n\to\infty} f(A_n)e_k = f(A)e_k$ for all $k \in \mathbb{N}$. Similarly $\lim_{n\to\infty} f(B_n)e_k = f(B)e_k$ for all $k \in \mathbb{N}$.

Let $m \in \mathbb{N}$. Then for all $n \in \mathbb{N}$ with $n > m$ we obtain by Proposition 2.4 that

$$\begin{aligned}\sum_{k=1}^{m} \|(f(A_n) - f(B_n))e_k\|_{\mathcal{H}}^2 &\leq \sum_{k=1}^{n} \|(f(A_n) - f(B_n))e_k\|_{\mathcal{H}}^2 = \|f(A_n) - f(B_n)\|_{\mathrm{HS}}^2 \\ &\leq L^2\, \|A_n - B_n\|_{\mathrm{HS}}^2 = L^2\, \|P_n\, C\, P_n\|_{\mathrm{HS}}^2 \leq L^2\, \|C\|_{\mathrm{HS}}^2.\end{aligned}$$

Now take the limit $n \to \infty$ to deduce that

$$\sum_{k=1}^{m} \|(f(A) - f(B))e_k\|_{\mathcal{H}}^2 \leq L^2\, \|C\|_{\mathrm{HS}}^2.$$

The limit $m \to \infty$ gives $\|f(A) - f(B)\|_{\mathrm{HS}}^2 \leq L^2\, \|C\|_{\mathrm{HS}}^2$ as required. □

In the next step we drop the assumption that f is bounded, but keep that $\mathcal{H}$ is separable.

Proposition 2.6. *Adopt the assumptions and notation of Theorem* 1.1*. Suppose in addition that the Hilbert space $\mathcal{H}$ is separable. Then $D(A) = D(B) \subset D(f(A)) = D(f(B))$ and the operator $f(A) - f(B)$ extends to a Hilbert–Schmidt operator, by abuse of notation still denoted by $f(A) - f(B)$, such that*

$$\|f(A) - f(B)\|_{\rm HS} \leq L\,\|C\|_{\rm HS}.$$

Proof. The equality $D(A) = D(B)$ is trivial.

For all $n \in \mathbb{N}$ define $\chi_n \colon \mathbb{R} \to \mathbb{R}$ by $\chi_n = (-n) \vee x \wedge n$. Then χ_n is Lipschitz continuous with Lipschitz constant 1. Hence the composition $f_n = \chi_n \circ f$ is Lipschitz continuous with Lipschitz constant M. Define $T_n = f_n(A) - f_n(B)$. It follows from Proposition 2.5 that $T_n \in \mathcal{L}_{\rm HS}(\mathcal{H})$ and $\|T_n\|_{\rm HS} \leq L\,\|C\|_{\rm HS}$. Hence the sequence $(T_n)_{n\in\mathbb{N}}$ is bounded in the Hilbert space $\mathcal{L}_{\rm HS}(\mathcal{H})$. Passing to a subsequence if necessary, there exists a $T \in \mathcal{L}_{\rm HS}(\mathcal{H})$ such that $\lim_{n\to\infty} T_n = T$ weakly in $\mathcal{L}_{\rm HS}(\mathcal{H})$. Then $\lim_{n\to\infty} T_n = T$ in the weak operator topology on $\mathcal{L}(\mathcal{H})$ and $\lim_{n\to\infty} T_n u = Tu$ weakly in $\mathcal{H}$ for all $u \in \mathcal{H}$

Now let $u \in D(A)$. Then $u \in D(f(A))$ by Lemma 2.1(a). So $\lim_{n\to\infty} f_n(A)u = f(A)u$ in $\mathcal{H}$ by Lemma 2.1(c). Similarly $\lim_{n\to\infty} f_n(B)u = f(B)u$. Hence $\lim_{n\to\infty} T_n u = (f(A) - f(B))u$ in $\mathcal{H}$. Therefore $Tu = (f(A) - f(B))u$ for all $u \in D(A)$ and $f(A)u = f(B)u + Tu$ for all $u \in D(A)$. Since $D(A)$ is a core for $f(B)$ by Lemma 2.1(b) and $f(A)$ is closed, it follows from Lemma 2.2 that $D(f(B)) \subset D(f(A))$ and $f(A)u = f(B)u + Tu$ for all $u \in D(f(A))$. Similarly $D(f(A)) \subset D(f(B))$. Hence $D(f(A)) = D(f(B))$. Moreover, T is an extension of $f(A) - f(B)$.

Finally, since $\lim_{n\to\infty} T_n = T$ weakly in $\mathcal{L}_{\rm HS}(\mathcal{H})$ one deduces that

$$\|T\|_{\rm HS} \leq \liminf_{n\to\infty} \|T_n\|_{\rm HS} \leq L\,\|C\|_{\rm HS}$$

as required. □

Finally we drop the assumption that $\mathcal{H}$ is separable.

Proof of Theorem 1.1. Since C is a compact operator, there exists a separable subspace $\mathcal{H}_0$ of $\mathcal{H}$ such that $C(\mathcal{H}_0) \subset \mathcal{H}_0$ and $Cu = 0$ for all $u \in \mathcal{H}_0^\perp$. Let U and V be the Cayley transforms of A and B. There exists a separable closed subspace $\mathcal{H}_1$ of $\mathcal{H}$ such that $\mathcal{H}_0 \subset \mathcal{H}_1$ and $\mathcal{H}_1$ is invariant under the four bounded operators U, V, U^* and V^*. Write $\mathcal{H}_2 = \mathcal{H}_1^\perp$. Then $\mathcal{H}_2$ is invariant under U and V. Let $P \colon \mathcal{H} \to \mathcal{H}_1$ be the orthogonal projection onto $\mathcal{H}_1$. Then the restriction of U to $\mathcal{H}_1$ is a unitary map from $\mathcal{H}_1$ onto $\mathcal{H}_1$. This corresponds to a self-adjoint operator A_1 in $\mathcal{H}_1$. Moreover, if $u \in D(A)$, then $Pu \in D(A_1)$ and $A_1 Pu = PAu$. Similarly one can define a self-adjoint operator A_2 in $\mathcal{H}_2$. Moreover, one can define similarly operators B_1 and B_2.

Since $A = B + C$ one deduces that $A_1 = B_1 + C$ and $A_2 = B_2$. Proposition 2.6 gives $D(A_1) = D(B_1) \subset D(f(A_1)) = D(f(B_1))$ and the operator $f(A_1) - f(B_1)$ extends to a Hilbert–Schmidt operator on $\mathcal{H}_1$, denoted by T_1, such that $\|T_1\|_{\rm HS} \leq L\,\|C\|_{\rm HS}$. Trivially $f(A_2) = f(B_2)$. Now $f(A) = f(A_1) \oplus f(A_2)$, with a similar decomposition for $f(B)$. So $D(f(A)) = D(f(B))$. Moreover, $f(A) - f(B) = (f(A_1) - f(B_1)) \oplus 0$. Hence the operator $T_1 \oplus 0$ extends $f(A) - f(B)$. Furthermore, $T \oplus 0$ is a Hilbert–Schmidt operator with $\|T \oplus 0\|_{\rm HS} \leq L\,\|C\|_{\rm HS}$. The proof of Theorem 1.1 is complete. □

3 Resolvent estimates

Very often one is in the situation that self-adjoint operators A and B do not differ by a Hilbert–Schmidt operator, but the difference of the resolvents $(A-\lambda)^{-1}-(B-\lambda)^{-1}$ is a Hilbert–Schmidt operator. Under an additional decay assumption on the function f we shall show that $f(A)-f(B)$ is a Hilbert–Schmidt operator and estimate the Hilbert–Schmidt norm in terms of the Hilbert–Schmidt norm of the difference of the resolvents.

Theorem 3.1. *Let A and B be two lower-bounded self-adjoint operators with lower bound $\rho \in \mathbb{R}$. Let $\lambda > -\rho$. Let $f\colon (0, \frac{1}{\lambda-\rho}] \to \mathbb{R}$ be a Lipschitz continuous function with Lipschitz constant L. Define $g\colon [-\rho,\infty) \to \mathbb{R}$ by $g(x) = f(\frac{1}{x+\lambda})$. Suppose that the difference of the resolvents $(A+\lambda\, I)^{-1}-(B+\lambda\, I)^{-1}$ is a Hilbert–Schmidt operator. Then $g(A)$ and $g(B)$ are bounded operators, their difference is a Hilbert–Schmidt operator and*

$$\|g(A)-g(B)\|_{\mathrm{HS}} \le L\, \|(A+\lambda)^{-1}-(B+\lambda)^{-1}\|_{\mathrm{HS}}.$$

Proof. Note that $g(A) = f((A+\lambda\, I)^{-1})$. We may extend f to a Lipschitz continuous function, again denoted by f, by taking it constant on $(-\infty,0]$ and constant on $(\frac{1}{\lambda-\rho},\infty)$. Then f is bounded, so $f((A+\lambda\, I)^{-1})$ is bounded. Similarly $g(B) = f((B+\lambda\, I)^{-1})$ is bounded. Then the theorem follows from Theorem 1.1 or Proposition 2.5. □

Corollary 3.2. *Let A and B be two lower-bounded self-adjoint operators with lower bound $\rho \in \mathbb{R}$. Let $\lambda > -\rho$. Let $g\colon [\rho,\infty) \to \mathbb{R}$ be a differentiable function and suppose that $L = \sup_{x\in[\rho,\infty)}(x+\lambda)^2\,|g'(x)| < \infty$. Suppose that the difference of the resolvents $(A+\lambda\, I)^{-1}-(B+\lambda\, I)^{-1}$ is a Hilbert–Schmidt operator. Then $g(A)$ and $g(B)$ are bounded operators, their difference is a Hilbert–Schmidt operator and*

$$\|g(A)-g(B)\|_{\mathrm{HS}} \le L\, \|(A+\lambda)^{-1}-(B+\lambda)^{-1}\|_{\mathrm{HS}}.$$

Proof. Define $f\colon (0,\frac{1}{\lambda-\rho}] \to \mathbb{R}$ by $f(t) = g(\frac{1}{t}-\lambda)$. Then $g(x) = f(\frac{1}{x+\lambda})$ for all $x \in [\rho,\infty)$. Moreover, $f'(t) = -\frac{1}{t^2}\, g'(\frac{1}{t}-\lambda) = -(x+\lambda)^2\, g'(x)$ for all $t \in (0,\frac{1}{\lambda-\rho}]$, where $x = \frac{1}{t}-\lambda$. Hence f is Lipschitz continuous with Lipschitz constant L. Now apply Theorem 3.1. □

4 A contractive iteration scheme

In this section we provide a sufficient condition to obtain a solution of a nonlinear map on a real Hilbert space via the Banach contraction theorem.

If $\mathcal{H}$ is a real Hilbert space, $A\colon \mathcal{H} \to \mathcal{H}^*$ is a map and $m > 0$, then A is called **strongly monotone** with **monotonicity constant** m if $\langle Au-Av, u-v\rangle_{\mathcal{H}^*\times\mathcal{H}} \ge m\,\|u-v\|_{\mathcal{H}}^2$ for all $u,v \in \mathcal{H}$. Note that then $\|Au-Av\|_{\mathcal{H}} \ge m\|u-v\|_{\mathcal{H}}$ and A is injective.

Theorem 4.1. *Let $\mathcal{H}$ be a real Hilbert space, $m > 0$ and $A\colon \mathcal{H} \to \mathcal{H}^*$ a strongly monotonous map with monotonicity constant m. Let $R > 0$ and let $\mathcal{B} = \{u \in \mathcal{H} : \|u\|_{\mathcal{H}} \le R\}$ be the closed ball centred at 0 and radius R. Suppose that the restriction $A|_{\mathcal{B}}$ is Lipschitz continuous with Lipschitz constant M. Let $J\colon \mathcal{H} \to \mathcal{H}^*$ denote the duality map. Fix $f \in \mathcal{H}^*$. Define $Q\colon \mathcal{B} \to \mathcal{H}$ by*

$$Qu = u - \frac{m}{M^2}\, J^{-1}(Au-f).$$

Then one has the following.

(a) *The map Q is a contraction with contraction constant $\sqrt{1 - \frac{m^2}{M^2}}$.*

(b) *Suppose $R \geq \frac{2}{m} \|A0 - f\|_{\mathcal{H}^*}$. Then Q maps $\mathcal{B}$ into itself.*

(c) *Suppose $R \geq \frac{2}{m} \|A0 - f\|_{\mathcal{H}^*}$. Then there exists a unique $u \in \mathcal{B}$ such that $Au = f$. Define $u_1 = 0$ and for all $n \in \mathbb{N}$ define $u_{n+1} = Qu_n$. Then $u = \lim_{n\to\infty} u_n$. Moreover,*

$$\|u\|_{\mathcal{H}} \leq \frac{1}{m} \|A0 - f\|_{\mathcal{H}^*}.$$

(d) *Let also $g \in \mathcal{H}^*$. Suppose $R \geq \frac{2}{m} \|A0 - f\|_{\mathcal{H}^*}$ and $R \geq \frac{2}{m} \|A0 - g\|_{\mathcal{H}^*}$. Then there exist unique $u, v \in \mathcal{H}$ such that $Au = f$ and $Av = g$. Furthermore, $\|u - v\|_{\mathcal{H}} \leq \frac{1}{m} \|f - g\|_{\mathcal{H}^*}$.*

Proof. '(a)'. Let $u, v \in \mathcal{B}$. Using the duality map J, one estimates

$$\begin{aligned}
\|Qu - Qv\|_{\mathcal{H}}^2 &= (u - v - \frac{m}{M^2} J^{-1}(Au - Av), u - v - \frac{m}{M^2} J^{-1}(Au - Av))_{\mathcal{H}} \\
&= \|u - v\|_{\mathcal{H}}^2 - 2\frac{m}{M^2}(J^{-1}(Au - Av), u - v)_{\mathcal{H}} + \frac{m^2}{M^4} \|J^{-1}(Au - Av)\|_{\mathcal{H}}^2 \\
&= \|u - v\|_{\mathcal{H}}^2 - 2\frac{m}{M^2}\langle Au - Av, u - v\rangle_{\mathcal{H}^*\times\mathcal{H}} + \frac{m^2}{M^4} \|Au - Av\|_{\mathcal{H}^*}^2 \\
&\leq \|u - v\|_{\mathcal{H}}^2 - 2\frac{m^2}{M^2}\|u - v\|_{\mathcal{H}}^2 + \frac{m^2}{M^2}\|u - v\|_{\mathcal{H}}^2 = (1 - \frac{m^2}{M^2})\|u - v\|_{\mathcal{H}}^2,
\end{aligned}$$

where we used the strong monotonicity and Lipschitz continuity in the last inequality.

'(b)'. Let $u \in \mathcal{B}$. Then if follows from Statement (a) that

$$\begin{aligned}
\|Qu\|_{\mathcal{H}} \leq \|Qu - Q0\|_{\mathcal{H}} + \|Q0\|_{\mathcal{H}} &\leq \sqrt{1 - \frac{m^2}{M^2}}\|u\|_{\mathcal{H}} + \frac{m}{M^2}\|A0 - f\|_{\mathcal{H}^*} \\
&\leq \Big(\sqrt{1 - \frac{m^2}{M^2}} + \frac{m^2}{2M^2}\Big)R \leq R.
\end{aligned}$$

'(c)'. Most follows from the Banach fixed point theorem. Since

$$\|f - A0\|_{\mathcal{H}^*} \|u\|_{\mathcal{H}} = \|Au - A0\|_{\mathcal{H}^*} \|u\|_{\mathcal{H}} \geq \langle Au - A0, u - 0\rangle_{\mathcal{H}^*\times\mathcal{H}} \geq m\|u\|_{\mathcal{H}}^2,$$

the estimate follows.

'(d)'. The existence follows from Statement (c). The monotonicity gives $m \|u-v\|_{\mathcal{H}}^2 \leq \langle Au-Av, u-v\rangle_{\mathcal{H}^*\times\mathcal{H}} = \langle f-g, u-v\rangle_{\mathcal{H}^*\times\mathcal{H}} \leq \|f-g\|_{\mathcal{H}^*} \|u-v\|_{\mathcal{H}}$ and hence $m \|u-v\|_{\mathcal{H}} \leq \|f-g\|_{\mathcal{H}^*}$. □

In [Zei] Section 25.4 and [GGZ] Theorem 3.4 in Subsection III.3.2 *global* Lipschitz continuity for A is demanded, but in the latter is at least indicated that local Lipschitz continuity suffices. The required radius of the ball $\mathcal{B}$ in [GGZ], however, is not optimal, and the proof is unnecessarily complicated. In general, *global* Lipschitz continuity is a severe restriction and, in general not fulfilled if A is not linear. In particular, the operator used in Proposition 5.14 is not globally Lipschitz.

5 An application in density functional theory

In this section we give an application of Corollary 3.2 via a Schrödinger–Poisson system used in electron transport theory. The main theorem of this section is as follows.

Theorem 5.1. *Let $d \in \{1, 2, 3\}$ and $\Omega \subset \mathbb{R}^d$ a bounded open set with Lipschitz boundary. Let $\varepsilon, \mathfrak{m} \colon \Omega \to \mathbb{R}^{d\times d}$ be bounded measurable functions with $\varepsilon(x)$ and $\mathfrak{m}(x)$ symmetric for all $x \in \Omega$. Let $\mu, \tilde{\mu} > 0$. Suppose that*

$$(\varepsilon(x)\xi, \xi)_{\mathbb{R}^d} \geq \mu \, \|\xi\|^2_{\mathbb{R}^d} \quad \text{and} \quad (\mathfrak{m}(x)\xi, \xi)_{\mathbb{R}^d} \geq \tilde{\mu} \, \|\xi\|^2_{\mathbb{R}^d}$$

for all $\xi \in \mathbb{R}^d$. Let $f \colon \mathbb{R} \to (0, \infty)$ be a differentiable and strictly decreasing function with f' locally bounded. Moreover, suppose that both $r \mapsto r^4 \, f(r)$ and $r \mapsto r^4 \, f'(r)$ are bounded on $[0, \infty)$. Then $f \colon \mathbb{R} \to f(\mathbb{R})$ is bijective and assume in addition that its inverse is locally Lipschitz. Let $D \subset \partial\Omega$ be closed. Fix $N > 0$.

Let $W^{1,2}_D(\Omega)$ be the $W^{1,2}(\Omega)$-closure of the set $\{u|_\Omega : u \in C^\infty(\mathbb{R}^d)$ and $\operatorname{supp} u \cap D = \emptyset\}$. Let $c_P > 0$. Suppose that

$$\|u\|^2_{L_2(\Omega)} \leq c_P \, \|\nabla u\|^2_{L_2(\Omega)}$$

for all $u \in W^{1,2}_D(\Omega)$. (So the space $W^{1,2}_D(\Omega)$ admits a Poincaré inequality.) For all $V \in L_2(\Omega, \mathbb{R})$ and $\psi, \varphi \in W^{1,2}_D(\Omega)$ it follows that $V \, \psi \, \overline{\varphi} \in L_1(\Omega)$. Define $\mathfrak{t}_V \colon W^{1,2}_D(\Omega) \times W^{1,2}_D(\Omega) \to \mathbb{C}$ by

$$\mathfrak{t}_V[\psi, \varphi] = \mathfrak{t}[\psi, \varphi] + \int_\Omega V \, \psi \, \overline{\varphi}.$$

Then one has the following.

(a) *For all $V \in L_2(\Omega, \mathbb{R})$ the sesquilinear form $\mathfrak{t}_V$ is closed, symmetric and lower-bounded. We denote by H the associated operator in case $V = 0$ and by $H \dotplus V$ the associated lower-bounded self-adjoint operator.*

(b) *For all $V \in L_2(\Omega, \mathbb{R})$ the operator $f(H \dotplus V)$ is nuclear.*

(c) *For all $V \in L_2(\Omega, \mathbb{R})$ there exists a unique $\mathcal{E}(V) \in \mathbb{R}$ such that*

$$\operatorname{tr} f(H \dotplus (V - \mathcal{E}(V) \, \mathbb{1}_\Omega)) = N.$$

(d) *For all $V \in L_2(\Omega, \mathbb{R})$ there exists a unique $\mathcal{N}(V) \in L_2(\Omega, \mathbb{R})$ such that*

$$\int_\Omega \mathcal{N}(V) \, W = \operatorname{tr}\big(M_W \, f(H \dotplus V - \mathcal{E}(V))\big)$$

for all $W \in L_\infty(\Omega)$, where M_W is the multiplication operator with W.

(e) *For all $V_0 \in L_2(\Omega, \mathbb{R})$ and $q \in (W^{1,2}_D(\Omega, \mathbb{R}))^*$ there exists a unique $V \in W^{1,2}_D(\Omega, \mathbb{R})$ such that*

$$\int_\Omega \varepsilon \nabla V \cdot \nabla W - (\mathcal{N}(V_0 + V), W)_{L_2(\Omega)} = \langle q, W \rangle_{(W^{1,2}_D(\Omega,\mathbb{R}))^* \times W^{1,2}_D(\Omega,\mathbb{R})}$$

for all $W \in W^{1,2}_D(\Omega, \mathbb{R})$. Write $\Psi(V_0, q) = V$.

(f) *If $V_0 \in L_2(\Omega, \mathbb{R})$ and $q \in (W^{1,2}_D(\Omega, \mathbb{R}))^*$, then*

$$\|\Psi(V_0, q)\|_{W^{1,2}_D(\Omega,\mathbb{R})} \leq \frac{1 + c_P}{\mu} \, \|q + \mathcal{N}(V_0)\|_{(W^{1,2}_D(\Omega))^*}.$$

(g) *If $V_0 \in L_2(\Omega, \mathbb{R})$, then*

$$\|\Psi(V_0, q) - \Psi(V_0, \tilde{q})\|_{W_D^{1,2}(\Omega)} \leq \frac{1 + c_P}{\mu} \|q - \tilde{q}\|_{(W_D^{1,2}(\Omega))^*}$$

for all $q, \tilde{q} \in (W_D^{1,2}(\Omega, \mathbb{R}))^*$.

(h) *For all $R > 0$ there is a $c > 0$ such that*

$$\|\Psi(V_0, q) - \Psi(V_1, \tilde{q})\|_{W_D^{1,2}(\Omega)} \leq c \|V_0 - V_1\|_{L_2} + \frac{1 + c_P}{\mu} \|q - \tilde{q}\|_{(W_D^{1,2}(\Omega))^*}$$

for all $V_0, V_1 \in L_2(\Omega, \mathbb{R})$ and $q, \tilde{q} \in (W_D^{1,2}(\Omega, \mathbb{R}))^*$ with $\|V_0\|_{L_2} \leq R$, $\|V_1\|_{L_2} \leq R$, $\|q\|_{(W_D^{1,2}(\Omega))^*} \leq R$ and $\|\tilde{q}\|_{(W_D^{1,2}(\Omega))^*} \leq R$.

The proof of Theorem 5.1 requires quite some preparation and the statements will be proved in separate lemmas and propositions in this section. Throughout this section we adopt the notation and assumptions of Theorem 5.1.

Define the sesquilinear form $\mathfrak{t} \colon W_D^{1,2}(\Omega) \times W_D^{1,2}(\Omega) \to \mathbb{C}$ by

$$\mathfrak{t}[\psi, \varphi] = \int_\Omega \mathfrak{m}^{-1} \nabla\psi \cdot \overline{\nabla\varphi}.$$

Then $\mathfrak{t}$ is a closed positive symmetric form. We define the unperturbed Schrödinger operator H on $L_2(\Omega)$ as the operator associated to the form $\mathfrak{t}$. Formally $H = -\operatorname{div}\big(\mathfrak{m}^{-1}\nabla\big)$ In semiconductor modelling $\mathfrak{m}$ describes the position dependent effective mass (modulo Planck's constant and a factor 2). Then H is a positive self-adjoint operator. The form domain $W_D^{1,2}(\Omega)$ gives the realisation of the operator H with homogeneous Dirichlet conditions on D and homogeneous Neumann conditions on $\partial\Omega \setminus D$. We refer to [ET] for more details of the spaces $W_D^{1,2}(\Omega)$.

We need for the sequel that the resolvent of H is a Hilbert–Schmidt operator, or equivalently that $(H+1)^{-1/2}$ belongs to the Schatten 4-class.

Proposition 5.2. $(H+1)^{-1/2} \in \mathcal{S}_4$.

Proof. Define $\mathfrak{l} \colon W^{1,2}(\Omega) \times W^{1,2}(\Omega) \to \mathbb{C}$ by $\mathfrak{l}[\psi, \varphi] = \int_\Omega \nabla\psi \cdot \overline{\nabla\varphi}$. Then there is a $c > 0$ such that $\mathfrak{l}[\psi] \leq c\, \mathfrak{t}[\psi]$ for all $\psi \in W_D^{1,2}(\Omega)$. If Δ_N is the Laplacian with Neumann boundary conditions, then $-\Delta_N$ is the operator associated with $\mathfrak{l}$. Let $\lambda_1 \leq \lambda_2 \leq \ldots$ be the eigenvalues of the operator H, repeated with multiplicity and let $\mu_1 \leq \mu_2 \leq \ldots$ be the eigenvalues of the operator $-\Delta_N$, repeated with multiplicity. Then the mini-max theorem gives $\mu_n \leq c\, \lambda_n$ for all $n \in \mathbb{N}$. The Weyl asymptotics give that there is a $c' > 0$ such that $\mu_n \geq c'\, n^{2/d}$ for large $n \in \mathbb{N}$. Since $d \leq 3$ this implies that $\sum_{n=1}^\infty \Big((\lambda_n + 1)^{-1/2}\Big)^4 < \infty$. □

In the sequel H is perturbed by a potential $V \in L_2(\Omega, \mathbb{R})$. We will prove a form bound with respect to $\mathfrak{t}$ in order to see that the form sum is well-defined.

Lemma 5.3. *There is a $\gamma > 0$ such that*

$$\Big| \int_\Omega V \psi\, \overline{\psi} \Big| \leq \frac{3}{4} (\mathfrak{t} + 1)[\psi] + \gamma \|V\|_{L_2}^4 \|\psi\|_{L_2}^2$$

uniformly for all $V \in L_2(\Omega, \mathbb{R})$ and $\psi \in W_D^{1,2}(\Omega)$.

Proof. Since Ω is Lipschitz, one has the continuous embedding $W_D^{1,2}(\Omega) \hookrightarrow L_6(\Omega)$, where we use that $d \leq 3$. Let c_1 be the embedding constant. Then

$$\begin{aligned}\Big| \int_\Omega V\psi\,\overline{\psi}\Big| &\leq \|V\|_{L_2}\|\psi\|_{L_4}^2 \leq \|V\|_{L_2}(\|\psi\|_{L_6}^2)^{\frac{3}{4}}(\|\psi\|_{L_2}^2)^{\frac{1}{4}} \leq c_1^{\frac{3}{2}}\,\|V\|_{L_2}(\|\psi\|_{W_D^{1,2}}^2)^{\frac{3}{4}}(\|\psi\|_{L_2}^2)^{\frac{1}{4}} \\ &\leq c_1^{\frac{3}{2}}\Big((\|\mathfrak{m}\|_{L_\infty}+1)(\mathfrak{t}+1)[\psi]\Big)^{\frac{3}{4}}\|V\|_{L_2}(\|\psi\|_{L_2}^2)^{\frac{1}{4}} \\ &\leq \frac{3}{4}(\mathfrak{t}+1)[\psi] + \frac{c_1^6\|V\|_{L_2}^4(\|\mathfrak{m}\|_{L_\infty}+1)^3}{4}\|\psi\|_{L_2}^2\end{aligned}$$

by Young's inequality. □

Throughout the remainder of this section we let $\gamma > 0$ be as in Lemma 5.3. For all $V \in L_2(\Omega,\mathbb{R})$ define the sesquilinear form $\mathfrak{t}_V \colon W_D^{1,2}(\Omega) \times W_D^{1,2}(\Omega) \to \mathbb{C}$ by

$$\mathfrak{t}_V[\psi,\varphi] = \mathfrak{t}[\psi,\varphi] + \int_\Omega V\,\psi\,\overline{\varphi}.$$

By Lemma 5.3 the form $\mathfrak{t}_V$ is symmetric, semibounded and closed. We denote the corresponding self-adjoint operator by $H \dotplus V$.

Lemma 5.4. *Let $R > 0$. Define $\lambda = 1 + \gamma\,R^4$. Let $V \in L_2(\Omega,\mathbb{R})$ with $\|V\|_{L_2} \leq R$. Then one has the following.*

(a) *The operator $H \dotplus V + \lambda$ is positive, invertible and $\|(H \dotplus V + \lambda)^{-1}\|_{L_2\to L_2} \leq 4$.*

(b) $\frac{1}{4}\,\mathfrak{t}[\psi] - \lambda\,\|\psi\|_{L_2}^2 \leq \mathfrak{t}_V[\psi] \leq \frac{7}{4}\,\mathfrak{t}[\psi] + \lambda\,\|\psi\|_{L_2}^2$ *for all* $\psi \in W_D^{1,2}(\Omega)$.

(c) $\|(H+1)^{1/2}(H \dotplus V + \lambda)^{-1/2}\| \leq 2$.

(d) $\|(H \dotplus V + \lambda)^{-2}\|_{\mathcal{S}_1}^{1/4} = \|(H \dotplus V + \lambda)^{-1/2}\|_{\mathcal{S}_4} \leq 2\|(H+1)^{-1/2}\|_{\mathcal{S}_4} < \infty$.

Proof. '(a)'. Let $\psi \in W_D^{1,2}(\Omega)$. Then

$$\mathfrak{t}_V[\psi] = \mathfrak{t}[\psi] + \int_\Omega V\psi\,\overline{\psi} \geq \mathfrak{t}[\psi] - \Big|\int_\Omega V\psi\,\overline{\psi}\Big| \geq \frac{1}{4}(\mathfrak{t}+1)[\psi] - \lambda\,\|\psi\|_{L_2}^2,$$

or, equivalently,

$$\mathfrak{t}_V[\psi] + \lambda\,\|\psi\|_{L_2}^2 \geq \frac{1}{4}(\mathfrak{t}+1)[\psi]. \tag{5.1}$$

This implies Statement (a).

'(b)'. This follows similarly.

'(c)'. It follows from (5.1) that

$$\|(H \dotplus V + \lambda)^{1/2}\psi\|_{L_2}^2 \geq \frac{1}{2}\,\|(H+1)^{1/2}\psi\|_{L_2}^2$$

for all $\psi \in W_D^{1,2}(\Omega)$. Now use [Kat] Theorem VI.2.23.

'(d)'. Since $(H \dotplus V + \lambda)^{-1/2} = (H+1)^{-\frac{1}{2}}\Big((H+1)^{\frac{1}{2}}(H \dotplus V + \lambda)^{-1/2}\Big)$, the statement follows from Statement (c) and Proposition 5.2. □

The form method gives that $D(H^{1/2}) = D(H \dotplus V + 1 + \gamma \, \|V\|_{L_2}^4)^{1/2}$ for all $V \in L_2(\Omega, \mathbb{R})$. Even more is valid. For all $V \in L_2(\Omega, \mathbb{R})$ let M_V be the self-adjoint operator in $L_2(\Omega)$ by multiplication with V.

Proposition 5.5. *Let $R > 0$. Define $\lambda = 1 + \gamma \, R^4$. Then there is a $c > 0$ such that for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \leq R$ the following is valid.*

(a) $D(H \dotplus V) = D(H)$.

(b) $D(H) \subset L_\infty(\Omega) \subset D(M_V)$.

(c) $H \dotplus V = H + M_V$.

(d) $\|(H \dotplus V + \lambda)^{-1}\|_{L_2 \to L_\infty} \leq c$.

Proof. Let S be the semigroup on L_2 generated by $-(H + \lambda)$. It follows from [AE] Theorem 4.4 together with Example 4.3 that there are $c, \omega > 0$ such that $\|S_t\|_{L_2 \to L_\infty} \leq c \, t^{-d/4} \, e^{\omega t}$ for all $t > 0$. Let $\rho \in \mathbb{R}$ with $\rho > \omega$ be such that $c \, R \, (\rho - \omega)^{-\frac{4-d}{4}} \, \Gamma(\frac{4-d}{4}) = \frac{1}{2}$. Let $\psi \in L_2$. Then a Laplace transform gives $(H + \lambda + \rho)^{-1} \psi \in L_\infty$, where we use that $d \leq 3$. In particular, $D(H) \subset D(M_V)$. Moreover,

$$\begin{aligned}
\|M_V \, (H + \lambda + \rho)^{-1} \psi\|_{L_2} &\leq \|V\|_{L_2} \int_0^\infty e^{-\rho t} \, \|S_t\|_{L_2 \to L_\infty} \, dt \, \|\psi\|_{L_2} \\
&\leq c \, \|V\|_{L_2} \, (\rho - \omega)^{-\frac{4-d}{4}} \, \Gamma(\frac{4-d}{4}) \, \|\psi\|_{L_2} \\
&\leq \frac{1}{2} \, \|\psi\|_{L_2}.
\end{aligned}$$

Therefore M_V is H-bounded with relative bound $\frac{1}{2}$. Then it follows from [Kat] Theorem V.4.3 that the operator $H + M_V$ is self-adjoint. Note that $D(H + M_V) = D(H)$. Let $\psi \in D(H)$. Then $\psi \in D(M_V)$. If $\varphi \in W^{1,2}_D(\Omega)$, then $\mathfrak{t}_V[\psi, \varphi] = \mathfrak{t}[\psi, \varphi] + (V \psi, \varphi)_{L_2} = (H\psi + V\psi, \varphi)_{L_2}$. Hence $\psi \in D(H \dotplus V)$ and $(H \dotplus V)\psi = H\psi + V\psi = (H + M_V)\psi$. We proved that $H \dotplus V$ is an extension of $H + M_V$. But both $H \dotplus V$ and $H + M_V$ are self-adjoint. Therefore $H \dotplus V = H + M_V$. In particular $D(H \dotplus V) = D(H) \subset L_\infty$.

Next

$$(H \dotplus V + \lambda + \rho)^{-1} \Big(1 + M_V \, (H + \lambda + \rho)^{-1}\Big) = (H + \lambda + \rho)^{-1}$$

and

$$(H \dotplus V + \lambda + \rho)^{-1} = (H + \lambda + \rho)^{-1} \, \Big(1 + M_V \, (H + \lambda + \rho)^{-1}\Big)^{-1}.$$

Therefore $\|(H \dotplus V + \lambda + \rho)^{-1}\|_{L_2 \to L_\infty} \leq 2 \|(H + \lambda + \rho)^{-1}\|_{L_2 \to L_\infty}$. $\square$

As a result we obtain a resolvent equation. Note that the multiplication operator in the next corollary is an unbounded operator in general.

Corollary 5.6. *Let $R > 0$. Define $\lambda = 1 + \gamma \, R^4$. Let $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R$ and $\|V\|_{L_2} \leq R$. Then $D(H \dotplus V + \lambda) \subset D(M_U)$ and*

$$(H \dotplus U + \lambda)^{-1} - (H \dotplus V + \lambda)^{-1} = -(H \dotplus U + \lambda)^{-1} \, M_{U-V} \, (H \dotplus V + \lambda)^{-1}.$$

Lemma 5.7. *Let $R > 0$. Define $\lambda = 1 + \gamma \, R^4$. Then one has the following.*

(a) *For all $k \in \{0, \ldots, 4\}$ there is a $c_k > 0$ such that $f(H \dotplus V)\psi \in D((H \dotplus V + \lambda)^k)$ for all $\psi \in L_2(\Omega)$ and $\|(H \dotplus V + \lambda)^k f(H \dotplus V)\|_{L_2 \to L_2} \le c_k$ for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \le R$.*

(b) *For all $k \in \{0, 1, 2\}$ there exists an $M_k > 0$ such that the operator*

$$(H \dotplus V + \lambda)^k f(H \dotplus V)$$

is nuclear and $\|(H \dotplus V + \lambda)^k f(H \dotplus V)\|_{\mathcal{S}_1} \le M_k$ for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \le R$.

Proof. '(a)'. The operator $H \dotplus V$ is self-adjoint and lower bounded by $-\gamma$ by Lemma 5.4(a). Define $g\colon \mathbb{R} \to \mathbb{R}$ by $g(r) = (r + \lambda)^k f(r)$. Then g is bounded on $[-\lambda, \infty)$ by the assumptions on f. Therefore the spectral theorem gives $\|(H \dotplus V + \lambda)^k f(H \dotplus V)\|_{L_2 \to L_2} \le \sup_{r \in [-\lambda, \infty)} |g(r)| = \sup_{r \in [-\lambda, \infty)} (r + \lambda)^k f(r)$.

'(b)'. Now

$$\begin{aligned} \|(H \dotplus V + \lambda)^k f(H \dotplus V)\|_{\mathcal{S}_1} &\le \|\big(H \dotplus V + \lambda)^{-2}\|_{\mathcal{S}_1} \, \|\big((H \dotplus V + \lambda)^{k+2} f(H \dotplus V)\|_{L_2 \to L_2} \\ &\le (2\|(H + 1)^{-1/2}\|_{\mathcal{S}_4})^4 \, c_{k+2}, \end{aligned}$$

where we used Lemma 5.4(d) and Statement (a). □

For all $W \in L_\infty(\Omega)$ we denote by M_W the multiplication operator on $L_2(\Omega)$ by multiplying with W. Let $V \in L_2(\Omega, \mathbb{R})$. Choosing $k = 0$ in Lemma 5.7(b) gives that $f(H \dotplus V)$ is trace class. Then

$$|\operatorname{tr}(M_W f(H \dotplus V))| \le \|M_W\|_{L_2 \to L_2} \operatorname{tr} |f(H \dotplus V)| \le \|W\|_{L_\infty(\Omega)} \operatorname{tr} f(H \dotplus V)$$

for all $W \in L_\infty(\Omega)$. Hence there is a unique $\mathcal{M}(V) \in L_1(\Omega, \mathbb{R})$ such that

$$\int_\Omega \mathcal{M}(V)\, W = \operatorname{tr}\big(M_W\, f(H \dotplus V)\big)$$

for all $W \in L_\infty(\Omega)$.

Proposition 5.8. *Let $R > 0$. Then there exists an $M > 0$ such that the following is valid.*

(a) *If $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \le R$, then $\mathcal{M}(V) \in L_2(\Omega, \mathbb{R})$ and $\|\mathcal{M}(V)\|_{L_2} \le M$.*

(b) *$\|\mathcal{M}(U) - \mathcal{M}(V)\|_{L_2} \le M\, \|U - V\|_{L_2}$ for all $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \le R$ and $\|V\|_{L_2} \le R$.*

Proof. '(a)'. Let $c_3 > 0$ be as in Lemma 5.7(a) and $c > 0$ as in Proposition 5.5(d). Write $\lambda = 1 + \gamma\, R^4$. Let $W \in L_\infty(\Omega)$. Then

$$\begin{aligned} \Big| \int_\Omega \mathcal{M}(V)\, W \Big| &= \Big| \operatorname{tr}\big(M_W\, f(H \dotplus V)\big) \Big| \\ &= \Big| \operatorname{tr}\Big(M_W\, (H \dotplus V + \lambda)^{-1} (H \dotplus V + \lambda)^3 f(H \dotplus V)\, (H \dotplus V + \lambda)^{-2}\Big) \Big| \\ &\le \|M_W\, (H \dotplus V + \lambda)^{-1}\|_{L_2 \to L_2} \cdot \\ &\qquad \cdot \|(H \dotplus V + \lambda)^3 f(H \dotplus V)\|_{L_2 \to L_2} \|(H \dotplus V + \lambda)^{-2}\|_{\mathcal{S}_1} \\ &\le c\, \|W\|_{L_2}\, c_3\, (2\|(H + 1)^{-1/2}\|_{\mathcal{S}_4})^4, \end{aligned}$$

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where we used Proposition 5.5(d), Lemma 5.7(a) and Lemma 5.4(d).

'(b)'. Write $\lambda = 1 + \gamma R^4$. Define the function $g \colon \mathbb{R} \to \mathbb{R}$ by $g(r) = (r+\lambda)^2 f(r)$. Let $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \le R$ and $\|V\|_{L_2} \le R$. Let $W \in L_\infty(\Omega)$. Then

$$\begin{aligned}\int_\Omega \mathcal{M}(V)\, W &= \operatorname{tr}\left(M_W\, f(H \dotplus V)\right) \\ &= \operatorname{tr}\Big(g(H \dotplus V)\,(H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus V + \lambda)^{-1}\Big)\end{aligned}$$

with a similar expression for U instead of V. Therefore

$$\begin{aligned}&\Big|\int_\Omega \Big(\mathcal{M}(U) - \mathcal{M}(V)\Big)\, W\Big| \\ &\quad= \Big|\operatorname{tr}\Big(g(H \dotplus U) - g(H \dotplus V)\Big)(H \dotplus U + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1} \\ &\qquad\quad + \operatorname{tr} g(H \dotplus V)\,\Big((H \dotplus U + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1} \\ &\qquad\qquad\qquad - (H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus V + \lambda)^{-1}\Big)\Big| \\ &\quad\le \|g(H \dotplus U) - g(H \dotplus V)\|_{\mathrm{HS}}\, \|(H \dotplus U + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}} \\ &\qquad + \|g(H \dotplus V)\|_{\mathrm{HS}}\, \|(H \dotplus U + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1} \\ &\qquad\qquad\qquad - (H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus V + \lambda)^{-1}\|_{\mathrm{HS}}.\end{aligned}$$

We estimate the two factors of the two terms.

First consider $\|g(H \dotplus U) - g(H \dotplus V)\|_{\mathrm{HS}}$. If $r \in [-\lambda, \infty)$, then

$$(r+\lambda)^2\, |g'(r)| = 2(r+\lambda)^3\, f(r) + (r+\lambda)^4\, f'(r).$$

Set

$$L = \sup_{r \in [-\lambda,\infty)} (r+\lambda)^2\, |g'(r)|.$$

The assumptions on the function f imply that $L < \infty$. Then Corollary 3.2 together with Corollary 5.6 give

$$\begin{aligned}&\|g(H \dotplus U) - g(H \dotplus V)\|_{\mathrm{HS}} \\ &\quad\le L\, \|(H \dotplus U + \lambda)^{-1} - (H \dotplus V + \lambda)^{-1}\|_{\mathrm{HS}} \\ &\quad= L\, \|(H \dotplus U + \lambda)^{-1}\, M_{U-V}\, (H \dotplus V + \lambda)^{-1}\|_{\mathrm{HS}} \\ &\quad\le \|(H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}}\, \|M_{U-V}\, (H \dotplus V + \lambda)^{-1}\|_{L_2 \to L_2} \\ &\quad\le (2\|(H+1)^{-1/2}\|_{\mathcal{S}_4})^2\, c\, \|U - V\|_{L_2},\end{aligned}$$

where we used Lemma 5.4(d) and $c > 0$ is as in Proposition 5.5(d).

Secondly and similarly

$$\|(H \dotplus U + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}} \le (2\|(H+1)^{-1/2}\|_{\mathcal{S}_4})^2\, c\, \|W\|_{L_2}.$$

Thirdly,

$$\|g(H \dotplus V)\|_{\mathrm{HS}} \leq \|g(H \dotplus V)\|_{\mathcal{S}_1}^{1/2}\, \|g(H \dotplus V)\|_{L_2 \to L_2}^{1/2} \leq c_2^{1/2}\, M_2^{1/2},$$

where c_2 and M_2 are as in Lemma 5.7.

Finally, using again Corollary 5.6 we obtain

$$\begin{aligned}
&\|(H \dotplus U + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1} - (H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus V + \lambda)^{-1}\|_{\mathrm{HS}} \\
&\quad \leq \|\Big((H \dotplus U + \lambda)^{-1} - (H \dotplus V + \lambda)^{-1}\Big) M_W\, (H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}} \\
&\qquad\quad + \|(H \dotplus V + \lambda)^{-1}\, M_W \Big((H \dotplus U + \lambda)^{-1} - (H \dotplus V + \lambda)^{-1}\Big)\|_{\mathrm{HS}} \\
&\quad \leq \|(H \dotplus U + \lambda)^{-1}\, M_{U-V}\, (H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}} \\
&\qquad\quad + \|(H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1}\, M_{U-V}\, (H \dotplus V + \lambda)^{-1}\|_{\mathrm{HS}}.
\end{aligned}$$

Now

$$\begin{aligned}
&\|(H \dotplus U + \lambda)^{-1}\, M_{U-V}\, (H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}} \\
&\qquad \leq \|(H \dotplus U + \lambda)^{-1}\|_{\mathrm{HS}}\, \|M_{U-V}\, (H \dotplus V + \lambda)^{-1}\|_{L_2 \to L_2} \cdot \\
&\qquad\qquad \cdot \|M_W\, (H \dotplus U + \lambda)^{-1}\|_{L_2 \to L_2} \\
&\qquad \leq (2\|(H+1)^{-1/2}\|_{\mathcal{S}_4})^2\, c^2\, \|U - V\|_{L_2}\, \|W\|_{L_2},
\end{aligned}$$

where we used Lemma 5.4(d) and $c > 0$ is as in Proposition 5.5. Similarly

$$\begin{aligned}
&\|(H \dotplus V + \lambda)^{-1}\, M_W\, (H \dotplus U + \lambda)^{-1}\, M_{U-V}\, (H \dotplus V + \lambda)^{-1}\|_{\mathrm{HS}} \\
&\qquad\qquad \leq (2\|(H+1)^{-1/2}\|_{\mathcal{S}_4})^2\, c^2\, \|U - V\|_{L_2}\, \|W\|_{L_2}.
\end{aligned}$$

Together we obtain that there is a $C > 0$ such that

$$\Big| \int_\Omega \Big(\mathcal{M}(U) - \mathcal{M}(V)\Big)\, W \Big| \leq C\, \|U - V\|_{L_2}\, \|W\|_{L_2}$$

for all $W \in L_\infty(\Omega)$ and $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R$ and $\|V\|_{L_2} \leq R$. Hence

$$\|\mathcal{M}(U) - \mathcal{M}(V)\|_{L_2} \leq C\, \|U - V\|_{L_2}$$

for all $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R$ and $\|V\|_{L_2} \leq R$, as required. □

The map $\mathcal{M}$ has the following monotonicity on the real Hilbert space $L_2(\Omega, \mathbb{R})$.

Proposition 5.9. *Let $U, V \in L_2(\Omega, \mathbb{R})$. Then $(\mathcal{M}(U) - \mathcal{M}(V), U - V)_{L_2} \leq 0$.*

Proof. We follow arguments given in [KNR]. First suppose that $U, V \in L_\infty(\Omega, \mathbb{R})$. There exists an orthonormal basis $(\psi_n)_{n \in \mathbb{N}}$ for $L_2(\Omega)$ and for all $n \in \mathbb{N}$ there is a $\lambda_n \in \mathbb{R}$ such that $(H \dotplus U)\psi_n = \lambda_n\, \psi_n$. Similarly there exists an orthonormal basis $(\varphi_n)_{n \in \mathbb{N}}$ for $L_2(\Omega)$ and for all $n \in \mathbb{N}$ there is a $\mu_n \in \mathbb{R}$ such that $(H \dotplus V)\varphi_n = \mu_n\, \varphi_n$.

Let $n, m \in \mathbb{N}$. Then $\psi_n \in D(H \dotplus U) = D(H) = D(H \dotplus V)$ by Proposition 5.5(a). Hence

$$((U - V)\psi_n, \varphi_m)_{L_2} = ((H \dotplus U - H \dotplus V)\psi_n, \varphi_m)_{L_2} = (\lambda_n - \mu_m)\, (\psi_n, \varphi_m)_{L_2}.$$

Then

$$\int_\Omega (U-V)\,\mathcal{M}(U) = \operatorname{tr}(M_{U-V}\, f(H \dotplus U) = \sum_{n=1}^\infty (M_{U-V}\, f(H \dotplus U)\psi_n, \psi_n)_{L_2}$$
$$= \sum_{n=1}^\infty f(\lambda_n)\,((U-V)\psi_n, \psi_n)_{L_2}$$
$$= \sum_{n,m=1}^\infty f(\lambda_n)\,((U-V)\psi_n, \varphi_m)_{L_2} (\varphi_m, \psi_n)_{L_2}$$
$$= \sum_{n,m=1}^\infty f(\lambda_n)\,(\lambda_n - \mu_m)\,|(\psi_n, \varphi_m)_{L_2}|^2.$$

Similarly

$$\int_\Omega (V-U)\,\mathcal{M}(V) = \sum_{n,m=1}^\infty f(\mu_m)\,(\mu_m - \lambda_n)\,|(\psi_n, \varphi_m)_{L_2}|^2.$$

Hence

$$\int_\Omega (U-V)\,\Big(\mathcal{M}(U) - \mathcal{M}(V)\Big) = \sum_{n,m=1}^\infty (f(\lambda_n) - f(\mu_m))\,(\lambda_n - \mu_m)\,|(\psi_n, \varphi_m)_{L_2}|^2 \le 0$$

since f is decreasing.

Now the proposition follows from Proposition 5.8(b) by density and continuity. □

If $V \in L_2(\Omega, \mathbb{R})$ and $t \in \mathbb{R}$, then $H \dotplus V - t = H + (V - t\,\mathbb{1}_\Omega)$ and $V - t\,\mathbb{1}_\Omega \in L_2(\Omega, \mathbb{R})$. Choosing $k = 0$ in Lemma 5.7(b) gives that $f(H \dotplus V - t)$ is trace class for all $V \in L_2(\Omega, \mathbb{R})$ and $t \in \mathbb{R}$.

Lemma 5.10. *For all $V \in L_2(\Omega, \mathbb{R})$ and $\widetilde{N} \in (0, \infty)$ there is a unique $t \in \mathbb{R}$ such that $\operatorname{tr}\big(f(H \dotplus V - t)\big) = \widetilde{N}$.*

Proof. Let $\lambda_1 \le \lambda_2 \le \ldots$ be the eigenvalues of the operator $H \dotplus V$, repeated with multiplicity. Then

$$\operatorname{tr}\big(f(H \dotplus V - t)\big) = \sum_{n=1}^\infty f(\lambda_n - t)$$

for all $t \in \mathbb{R}$. This series is absolutely convergent for each $t \in \mathbb{R}$. Since f is continuous and strictly decreasing, it follows from the Lebesgue dominated convergence theorem that $t \mapsto \operatorname{tr}\big(f(H \dotplus V - t)\big)$ is continuous and strictly increasing.

Because $f(0) > 0$ one deduces that $\lim_{t\to\infty} \operatorname{tr}\big(f(H \dotplus V - t)\big) = \infty$. Using again the Lebesgue dominated convergence theorem it follows that $\lim_{t\to-\infty} \operatorname{tr}\big(f(H \dotplus V - t)\big) = 0$. Then the existence follows. □

For all $V \in L_2(\Omega, \mathbb{R})$ we define the **Fermi level** $\mathcal{E}(V) = t$, where $t \in \mathbb{R}$ is such that

$$\operatorname{tr}\big(f(H \dotplus V - t)\big) = N.$$

Recall that N is fixed in Theorem 5.1. We next prove that the function $V \mapsto \mathcal{E}(V)$ is locally bounded.

Proposition 5.11. *For all $R > 0$ there exists an $M > 0$ such that $|\mathcal{E}(V)| \leq M$ for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \leq R$.*

Proof. The proof is a modification of the proof of Lemma 5.10. Write $\lambda = 1 + \gamma R^4$. For all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \leq R$ let $\lambda_1^{(V)} \leq \lambda_2^{(V)} \leq \ldots$ be the eigenvalues of the operator $H \dot{+} V$, repeated with multiplicity. Then the mini-max theorem together with the form bounds of Lemma 5.4(b) gives

$$\tfrac{1}{4} \lambda_n^{(0)} - \lambda \leq \lambda_n^{(V)} \leq \tfrac{7}{4} \lambda_n^{(0)} + \lambda$$

for all $n \in \mathbb{N}$. Let $t \in \mathbb{R}$. Since f is decreasing one estimates

$$\sum_{n=1}^{\infty} f(\tfrac{7}{4} \lambda_n^{(0)} + \lambda - t) \leq \sum_{n=1}^{\infty} f(\lambda_n^{(V)} - t) \leq \sum_{n=1}^{\infty} f(\tfrac{1}{4} \lambda_n^{(0)} - \lambda - t).$$

Arguing as in the proof of Lemma 5.10 there are $T, \widetilde{T} \in \mathbb{R}$ such that

$$\sum_{n=1}^{\infty} f(\tfrac{7}{4} \lambda_n^{(0)} + \lambda - T) = N = \sum_{n=1}^{\infty} f(\tfrac{1}{4} \lambda_n^{(0)} - \lambda - \widetilde{T}).$$

Then $T \geq \mathcal{E}(V) \geq \widetilde{T}$. □

Define the **particle density** $\mathcal{N} \colon L_2(\Omega, \mathbb{R}) \to L_2(\Omega, \mathbb{R})$ by

$$\mathcal{N}(V) = \mathcal{M}(V - \mathcal{E}(V) \, \mathbb{1}_\Omega).$$

So

$$\int_\Omega \mathcal{N}(V) \, W = \operatorname{tr}\big(M_W \, f(H \dot{+} V - \mathcal{E}(V))\big)$$

and

$$\int_\Omega \mathcal{N}(V) = \operatorname{tr} f(H \dot{+} V - \mathcal{E}(V)) = N \tag{5.2}$$

for all $V \in L_2(\Omega, \mathbb{R})$ and $W \in L_\infty(\Omega)$. We next prove that Proposition 5.8(b) remains valid if $\mathcal{M}$ is replaced by $\mathcal{N}$. This was proved before in [KR2] Section 4.

Proposition 5.12. *Let $R > 0$. Then there exists an $M > 0$ such that*

$$\|\mathcal{N}(U) - \mathcal{N}(V)\|_{L_2} \leq M \, \|U - V\|_{L_2}$$

for all $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R$ and $\|V\|_{L_2} \leq R$.

Proof. Using Propositions 5.11 and 5.8(b) it suffices to show that there is an $M > 0$ such that $|\mathcal{E}(U) - \mathcal{E}(V)| \leq M \, \|U - V\|_{L_2}$ for all $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R$ and $\|V\|_{L_2} \leq R$.

For all $V \in L_2(\Omega, \mathbb{R})$ let $\lambda_1^{(V)} \leq \lambda_2^{(V)} \leq \ldots$ be the eigenvalues of the operator $H \dot{+} V$, repeated with multiplicity. Then the mini-max theorem together with the form bounds of Lemma 5.4(b) gives

$$\tfrac{1}{4} \lambda_1^{(0)} - \lambda \leq \lambda_1^{(V)} \leq \tfrac{7}{4} \lambda_1^{(0)} + \lambda$$

for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \leq R$, where $\lambda = 1 + \gamma R^4$. By Proposition 5.11 there is an $M_1 > 0$ such that $|\mathcal{E}(V)| \leq M_1$ for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \leq R$. Since f is locally bounded, there is an $M_2 > 0$ such that $f(\lambda_1^{(V)} - \mathcal{E}(V)) \leq M_2$ for all $V \in L_2(\Omega, \mathbb{R})$ with $\|V\|_{L_2} \leq R$. By the assumptions on f there is an $L > 0$ such that $|t - s| \leq L\,|f(t) - f(s)|$ for all $t, s \in \mathbb{R}$ with $f(t) \in [-M_2, M_2]$ and $f(s) \in [-M_2, M_2]$. By Proposition 5.8(b) there is a $c > 0$ such that

$$\|\mathcal{M}(U) - \mathcal{M}(V)\|_{L_2} \leq c\,\|U - V\|_{L_2}$$

for all $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R + M_1\,|\Omega|^{1/2}$ and $\|V\|_{L_2} \leq R + M_1\,|\Omega|^{1/2}$.

Now let $U, V \in L_2(\Omega, \mathbb{R})$ with $\|U\|_{L_2} \leq R$ and $\|V\|_{L_2} \leq R$. Without loss of generality we may assume that $\mathcal{E}(V) \geq \mathcal{E}(U)$. Since f is decreasing one deduces that

$$f(\lambda_n^{(V)} - \mathcal{E}(V)) - f(\lambda_n^{(V)} - \mathcal{E}(U)) \geq 0$$

for all $n \in \mathbb{N}$. Consequently

$$\begin{aligned}
\operatorname{tr} f(H \dot{+} V - \mathcal{E}(V)) &- \operatorname{tr} f(H \dot{+} V - \mathcal{E}(U)) \\
&= \sum_{n=1}^{\infty} \Big(f(\lambda_n^{(V)} - \mathcal{E}(V)) - f(\lambda_n^{(V)} - \mathcal{E}(U)) \Big) \\
&\geq |f(\lambda_1^{(V)} - \mathcal{E}(V)) - f(\lambda_1^{(V)} - \mathcal{E}(U))| \\
&\geq L^{-1}\,|(\lambda_1^{(V)} - \mathcal{E}(V)) - (\lambda_1^{(V)} - \mathcal{E}(U))| \\
&= L^{-1}\,|\mathcal{E}(U) - \mathcal{E}(V)|.
\end{aligned}$$

On the other hand,

$$\operatorname{tr} f(H \dot{+} V - \mathcal{E}(V)) = N = \operatorname{tr} f(H \dot{+} U - \mathcal{E}(U))$$

and hence

$$\begin{aligned}
\operatorname{tr} f(H \dot{+} V - \mathcal{E}(V)) &- \operatorname{tr} f(H \dot{+} V - \mathcal{E}(U)) \\
&= |\operatorname{tr} f(H \dot{+} U - \mathcal{E}(U)) - \operatorname{tr} f(H \dot{+} V - \mathcal{E}(U))| \\
&= \Big| \int_\Omega \Big(\mathcal{M}(U - \mathcal{E}(U)) - \mathcal{M}(V - \mathcal{E}(U)) \Big) \Big| \\
&\leq |\Omega|^{1/2}\,\|\mathcal{M}(U - \mathcal{E}(U)) - \mathcal{M}(V - \mathcal{E}(U))\|_{L_2} \\
&\leq c\,|\Omega|^{1/2}\,\|U - V\|_{L_2}
\end{aligned}$$

from which the theorem follows. □

Also Proposition 5.9 is valid for $\mathcal{N}$ instead of $\mathcal{M}$.

Proposition 5.13. *Let $U, V \in L_2(\Omega, \mathbb{R})$. Then $(\mathcal{N}(U) - \mathcal{N}(V), U - V)_{L_2} \leq 0$.*

Proof. Using (5.2) and Proposition 5.9 one deduces that

$$\begin{aligned}
&(\mathcal{N}(U) - \mathcal{N}(V), U - V)_{L_2} \\
&\quad = (\mathcal{N}(U) - \mathcal{N}(V), (U - \mathcal{E}(U)\,\mathbb{1}_\Omega) - (V - \mathcal{E}(V)\,\mathbb{1}_\Omega))_{L_2} \\
&\quad = ((\mathcal{M}(U - \mathcal{E}(U)\,\mathbb{1}_\Omega) - \mathcal{M}(V - \mathcal{E}(V)\,\mathbb{1}_\Omega), (U - \mathcal{E}(U)\,\mathbb{1}_\Omega) - (V - \mathcal{E}(V)\,\mathbb{1}_\Omega))_{L_2} \leq 0
\end{aligned}$$

as required. □

We next show that for all $V_0 \in L_2(\Omega, \mathbb{R})$ and $q \in (W^{1,2}_D(\Omega, \mathbb{R}))^*$ there is a $V \in W^{1,2}_D(\Omega)$ such that

$$-\nabla \cdot \varepsilon \nabla V = q + \mathcal{N}(V_0 + V)$$

in a weak sense.

Proposition 5.14. *Let $V_0 \in L_2(\Omega, \mathbb{R})$. Write $\mathcal{H} = W^{1,2}_D(\Omega, \mathbb{R})$. Define the map $A_0 \colon \mathcal{H} \to \mathcal{H}^*$ by*

$$\langle A_0 V, W\rangle_{\mathcal{H}^* \times \mathcal{H}} = \int_\Omega \varepsilon \nabla V \cdot \nabla W - (\mathcal{N}(V_0 + V), W)_{L_2(\Omega)}.$$

Then one has the following.

(a) *The operator A_0 is strongly monotone with monotonicity constant $\mu\,(1 + c_P)^{-1}$.*

(b) *For all $R > 0$ there exists a $C > 0$ such that*

$$\|A_0 U - A_0 V\|_{\mathcal{H}^*} \le C\,\|U - V\|_{\mathcal{H}}$$

for all $U, V \in \mathcal{H}$ with $\|U\|_{\mathcal{H}} \le R$ and $\|V\|_{\mathcal{H}} \le R$.

(c) *For all $q \in \mathcal{H}^*$ there is a unique $V \in \mathcal{H}$ such that*

$$\langle A_0 V, W\rangle_{\mathcal{H}^* \times \mathcal{H}} = \langle q, W\rangle_{\mathcal{H}^* \times \mathcal{H}}$$

for all $W \in \mathcal{H}$. It follows that $\|V\|_{\mathcal{H}} \le \frac{1+c_P}{\mu}\,\|q + \mathcal{N}(V_0)\|_{\mathcal{H}^*}$.

Proof. '(a)'. Let $U, V \in \mathcal{H}$. Then

$$\begin{aligned}
&\langle A_0 U - A_0 V, U - V\rangle_{\mathcal{H}^* \times \mathcal{H}} \\
&\qquad \ge \mu \int_\Omega |\nabla(U - V)|^2 - (\mathcal{N}(V_0 + U) - \mathcal{N}(V_0 + V), (V_0 + U) - (V_0 + V))_{L_2} \\
&\qquad \ge \mu\,(1 + c_P)^{-1} \|U - V\|^2_{\mathcal{H}},
\end{aligned}$$

where we used Proposition 5.13.

'(b)'. This follows from Proposition 5.12 and the boundedness of the coefficient function ε.

'(c)'. This follows immediately from the previous statements and Theorem 4.1. □

Write $\Psi(V_0, q) = V$ if V_0, q and V are as in Proposition 5.14(c).

Proof of Theorem 5.1(h). If follows from Theorem 4.1(d) that

$$\|\Psi(V_0, q) - \Psi(V_0, \tilde{q})\|_{W^{1,2}_D(\Omega)} \le \frac{1 + c_P}{\mu}\,\|q - \tilde{q}\|_{(W^{1,2}_D(\Omega))^*}.$$

Hence it remains to estimate $\|\Psi(V_0, q) - \Psi(V_1, q)\|_{W^{1,2}_D(\Omega)}$. Write $\mathcal{H} = W^{1,2}_D(\Omega, \mathbb{R})$. Define the maps $A_0, A_1 \colon \mathcal{H} \to \mathcal{H}^*$ by

$$\langle A_0 V, W\rangle_{\mathcal{H}^* \times \mathcal{H}} = \int_\Omega \varepsilon \nabla V \cdot \nabla W - (\mathcal{N}(V_0 + V), W)_{L_2(\Omega)} \quad \text{and}$$

$$\langle A_1 V, W\rangle_{\mathcal{H}^* \times \mathcal{H}} = \int_\Omega \varepsilon \nabla V \cdot \nabla W - (\mathcal{N}(V_1 + V), W)_{L_2(\Omega)}.$$

Write $m = \frac{\mu}{1+c_P}$. Let

$$R = \frac{2}{m} \max\{\|q + \mathcal{N}(V_0)\|_{\mathcal{H}^*}, \|q + \mathcal{N}(V_1)\|_{\mathcal{H}^*}\}.$$

By Proposition 5.14(b) there exists an $M > 0$ such that

$$\|A_0 U - A_0 V\|_{\mathcal{H}^*} \le M \, \|U - V\|_{\mathcal{H}} \quad \text{and} \quad \|A_1 U - A_1 V\|_{\mathcal{H}^*} \le M \, \|U - V\|_{\mathcal{H}}$$

for all $U, V \in \mathcal{H}$ with $\|U\|_{\mathcal{H}} \le R$ and $\|V\|_{\mathcal{H}} \le R$. By Proposition 5.12 there exists a $c > 0$ such that

$$\|\mathcal{N}(U) - \mathcal{N}(V)\|_{L_2} \le c \, \|U - V\|_{L_2}$$

for all $U, V \in L_2(\Omega, \mathbb{R})$ such that $\|U\|_{L_2} \le R + \|V_0\|_{L_2} + \|V_1\|_{L_2}$ and $\|V\|_{L_2} \le R + \|V_0\|_{L_2} + \|V_1\|_{L_2}$. Let $J \colon \mathcal{H} \to \mathcal{H}^*$ be the duality map. Define $Q_0, Q_1 \colon \{U \in \mathcal{H} : \|U\|_{\mathcal{H}} \le R\} \to \mathcal{H}$ by

$$Q_0 U = U - \frac{m}{M^2} \, J^{-1}(A_0 U - q) \quad \text{and} \quad Q_1 U = U - \frac{m}{M^2} \, J^{-1}(A_1 U - q). \tag{5.3}$$

Now we estimate $\|\Psi(V_0, q) - \Psi(V_1, q)\|_{W^{1,2}_D(\Omega)}$. Write $U = \Psi(V_0, q)$ and $V = \Psi(V_1, q)$. Then $\|U\|_{L_2} \le R$ and $\|V\|_{L_2} \le R$ by Proposition 5.14(c). Moreover, $Q_0 U = U$ and $Q_1 V = V$. Using Proposition 5.14(a) and Theorem 4.1(a) one estimates

$$\begin{aligned} \|U - V\|_{\mathcal{H}} &= \|Q_0 U - Q_1 V\|_{\mathcal{H}} = \|Q_0 U - Q_0 V\|_{\mathcal{H}} + \|Q_0 V - Q_1 V\|_{\mathcal{H}} \\ &\le \sqrt{1 - \frac{m^2}{M^2}} \, \|U - V\|_{\mathcal{H}} + \frac{m}{M^2} \, \|J^{-1}(\mathcal{N}(V_0 + V) - \mathcal{N}(V_1 + V))\|_{\mathcal{H}}. \end{aligned}$$

Rearrangement gives

$$\begin{aligned} \|U - V\|_{\mathcal{H}} &\le \Big(1 - \sqrt{1 - \frac{m^2}{M^2}}\Big)^{-1} \, \frac{m}{M^2} \, \|\mathcal{N}(V_0 + V) - \mathcal{N}(V_1 + V)\|_{\mathcal{H}^*} \\ &\le \Big(1 - \sqrt{1 - \frac{m^2}{M^2}}\Big)^{-1} \, \frac{m}{M^2} \, \|I\|_{L_2 \to \mathcal{H}^*} \, \|\mathcal{N}(V_0 + V) - \mathcal{N}(V_1 + V)\|_{L_2} \\ &\le \Big(1 - \sqrt{1 - \frac{m^2}{M^2}}\Big)^{-1} \, \frac{m}{M^2} \, \|I\|_{L_2 \to \mathcal{H}^*} \, c \, \|V_0 - V_1\|_{L_2} \end{aligned}$$

as required. □

Finally we consider regularity of the solutions under some weak additional assumptions. For all $p \in (1, \infty)$ let $W^{1,p}_D(\Omega)$ be the $W^{1,p}(\Omega)$-closure of the set

$$\{u|_\Omega : u \in C^\infty(\mathbb{R}^d) \text{ and } \operatorname{supp} u \cap D = \emptyset\}.$$

Let p' be the dual exponent of p. Define $W^{-1,p'}_D(\Omega)$ to be the dual space of $W^{1,p}_D(\Omega)$.

Theorem 5.15. *Let* $V_0 \in L_2(\Omega, \mathbb{R})$*,* $p \in [2, \infty]$*, and* $q \in W^{-1,p}_D(\Omega, \mathbb{R})$*.*

(a) *If* $p > d$*, then* $\Psi(V_0, q) \in L_\infty(\Omega)$*.*

(b) *If* $2 < p \le d = 3$*, then* $\Psi(V_0, q) \in L_{p^*}(\Omega)$*, where* $\frac{1}{p^*} = \frac{1}{p} - \frac{1}{3}$*.*

(c) *Suppose $p > d$. Under a measure theoretic condition of the relative boundary of D in $\partial\Omega$ (see [ER] Assumption (III) in Theorem 1.1) it follows that $\Psi(V_0, q)$ is Hölder continuous for all $V_0 \in L_2(\Omega, \mathbb{R})$ and $q \in W_D^{-1,p}(\Omega)$.*

(d) *Suppose that $D = \partial\Omega$ and that the coefficient function ε is Lipschitz continuous. Further suppose that Ω is of class $C^{1,1}$ or convex. Then $\Psi(V_0, q) \in W^{2,2}(\Omega)$ if $q \in L_2(\Omega, \mathbb{R})$.*

Proof. The Sobolev embedding theorem gives $L_2(\Omega) \subset W_D^{-1,6}(\Omega)$. Write $\tilde{p} = \min(p, 6)$ and $V = \Psi(V_0, q)$. Then $q + \mathcal{N}(V_0 + V) \in W_D^{-1,\tilde{p}}(\Omega)$. Moreover,

$$\int_\Omega \varepsilon \nabla V \cdot \nabla W = \langle q + \mathcal{N}(V_0 + V), W\rangle_{\mathcal{D}'(\Omega)\times\mathcal{D}(\Omega)} \tag{5.4}$$

for all $W \in C_c^\infty(\Omega)$.

'(a)'. Now $\tilde{p} > d$ and [Sta] Théorème 4.2(a) implies that $V \in L_\infty(\Omega)$.

'(b)'. Now $\tilde{p} = p$ and one can use [Sta] Théorème 4.2(b).

'(c)'. See [ER] Theorem 1.1.

'(d)'. We use (5.4). Then the regularity follows from [Gri] Theorem 2.2.2.3 in case Ω is of class $C^{1,1}$ and from [Gri] Theorem 3.2.1.2 in case Ω is convex. □

Theorem 5.16. *Suppose that the set D is a $(d-1)$-set in the sense of Jonsson–Wallin ([JW] Chapter II). Then there exists a $p > 2$ such that $\Psi(V_0, q) \in W_D^{1,p}(\Omega)$ for all $V_0 \in L_2(\Omega, \mathbb{R})$ and $q \in W_D^{-1,p}(\Omega)$.*

Proof. This follows from [HJKR] Theorem 5.6. □

If $V_0 \in L_2(\Omega, \mathbb{R})$ and $q \in (W_D^{1,2}(\Omega, \mathbb{R}))^*$, then the solution $\Psi(V_0, q)$ of the Schrödinger–Poisson system obtained in Theorem 5.1(e), or Proposition 5.14(c), is constructed via a contraction in Theorem 4.1(c). Explicitly, if Q_0 is as in (5.3), $U_1 = 0$ and inductively $U_{n+1} = Q_0 U_n$ for all $n \in \mathbb{N}$, then $\Psi(V_0, q) = \lim_{n\to\infty} U_n$ in $W_D^{1,2}(\Omega)$. We do not know whether the convergence is valid in any of the spaces mentioned in Theorems 5.15 and 5.16.

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