Weierstraß-Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Convexity of trace functionals and Schrödinger operators

Dedicated to M. Sh. Birman on the occasion of his 75th birthday.

Hans–Christoph Kaiser, Hagen Neidhardt, Joachim Rehberg

submitted: 17th December 2003

Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstr. 39
D-10117 Berlin
Germany

E–Mail: kaiser@wias-berlin.de
neidhardt@wias-berlin.de
rehberg@wias-berlin.de

No. 835
Berlin 2003

2000 *Mathematics Subject Classification.* 47H05, 46T20, 47B10, 47F05.

Key words and phrases. trace functionals, convexity, monotonicity, double Stieltjes operator integrals, spectral asymptotics, generalized Fermi level, density–functional theory.

Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D — 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

Let H be a semi–bounded self–adjoint operator in a separable Hilbert space. For a certain class of positive, continuous, decreasing, and convex functions F we show the convexity of trace functionals $\mathrm{tr}(F(H + U - \varepsilon(U))) - \varepsilon(U)$, where U is a bounded self–adjoint operator on H and $\varepsilon(U)$ is a normalizing real function—the Fermi level—which may be identical zero. If additionally F is continuously differentiable, then the corresponding trace functional is Fréchet differentiable and there is an expression of its gradient in terms of the derivative of F. The proof of the differentiability of the trace functional is based upon Birman and Solomyak's theory of double Stieltjes operator integrals. If, in particular, H is a Schrödinger–type operator and U a real–valued function, then the gradient of the trace functional is the quantum mechanical expression of the particle density with respect to an equilibrium distribution function $f = -F'$. Thus, the monotonicity of the particle density in its dependence on the potential U of Schrödinger's operator—which has been understood since the late 1980s—follows as a special case.

2000 Mathematics Subject Classification: 47H05, 46T20, 47B10, 47F05.

2003 Physics and Astronomy Classification Scheme (PACS): 05.30.-d

Key words and phrases: trace functionals, convexity, monotonicity, double Stieltjes operator integrals, spectral asymptotics, generalized Fermi level, density–functional theory.

Contents

1 Introduction

In the semi–classical approximation the density of electrons and holes in a two–band bulk semiconductor depends continuously and monotone on the chemical potential of electrons and holes, respectively. This behaviour of the charge densities ensures the unique solvability of Poisson's equation for the electrostatic potential, see e.g. [9, 10, 24] and the references cited there.

In quantum semiconductor structures like resonant tunneling diodes and quantum well lasers the semi–classical approximation and its underlying assumption, that electrons and holes can move freely in all space directions, is not valid anymore. Instead, in a quantum well a quantization of energy levels takes place, see e.g. [7, 27]. The electron density in quasi low–dimensional systems, such as quantum–wells, –wires, and –dots in the infinitely high barriers limit, is obtained by solving an eigenvalue problem

$$(H + U)\psi_j(U) = \lambda_j(U)\psi_j(U)$$

for an appropriate Hamiltonian $H+U$ with pure point spectrum on a space of square integrable functions. More precisely, the electron density is given by

$$\sum_{j\in\mathbf{N}} f\left(\lambda_j(U) - \varepsilon(U)\right) \left|\psi_j(U)(x)\right|^2,$$

where f is the thermodynamic equilibrium distribution function for the system and ε is the quasi–Fermi potential which in general also depends on U. The shift $\varepsilon(U)$ normalizes the trace of $f\left(H + U - \varepsilon(U)\right)$ in such a way that $f\left(H + U - \varepsilon(U)\right)$ becomes a density matrix. In this paper we normalize to 1, though other conventions are also common. In semiconductor physics—H being a one–electron, effective mass Hamiltonian in Ben–Daniel–Duke form—one often chooses the total number of undistinguishable electrons in the system as normalizing condition. If the thermodynamic equilibrium distribution function f is smooth enough, strictly and sufficiently rapidly decreasing, then the electron density depends—as in the semi–classical approximation—continuously and anti–monotone on the potential of the Hamiltonian, which is, up to the normalizing shift, the negative chemical potential. This fact has been observed in 1990 independently by Caussignac et al. [6] and Nier [21] for the spatially one–dimensional case. In [22, 12, 13, 14, 15] the monotonicity result for the electron density has been extended to larger classes of thermodynamic equilibrium distribution functions f, to two and three space dimensions (that means to quantum wires and quantum dots) including the case of quantum heterostructures with mixed boundary conditions. As in the semi–classical approximation the monotonicity result for the electron and hole density has been used to prove existence and uniqueness of solutions for the corresponding non–linear Poisson equation, then usually addressed as Schrödinger–Poisson system [6, 21, 22, 12, 13, 14, 15]. Even more, one obtains existence and conditional uniqueness of solutions for the Euler equations of density functional theory—in local density approximation—, the so called Kohn–Sham system [14, 15].

In this paper we generalize the monotonicity result for the density to abstract quantum systems with an unperturbed Hamiltonian H which has pure point spectrum. Making minimal requirements on the continuity and the decay of the thermodynamic equilibrium distribution function f we prove that the density matrix $f\left(H+U-\varepsilon(U)\right)$ is the negative gradient of the convex functional

$$\operatorname{tr}\left(F\left(H+U-\varepsilon(U)\right)\right)-\varepsilon(U), \qquad F(t) \stackrel{\text{def}}{=} \int_t^\infty f(s)\,\mathrm{d}s,$$

where U is any bounded self–adjoint perturbation of H, see Theorem 33.

Our investigation uses a result by J. v. Neumann about the convexity of certain trace functionals, see Proposition 16. The differentiability of trace functionals $\operatorname{tr}\left(F(H+U)\right)$ with respect to U follows from Birman and Solomyak's theory of double Stieltjes operator integrals, see Proposition 20.

If the underlying Hilbert space is a space of square integrable functions and U is induced by an essentially bounded, real–valued function u, then the corresponding density matrices can be represented by the non–negative, integrable functions. The dependence of these functions on u is anti–monotone and continuous, see Corollary 37. This result covers, in particular, earlier ones by Caussignac et al. [6] and Nier [21]. In the framework of [6, 21] H is the kinetic energy part of a one–dimensional Schrödinger operator on a bounded interval; homogeneous Dirichlet boundary conditions ensure the discreteness of the spectrum.

Maz'ya et al. give necessary and sufficient conditions for the discreteness and positivity of the spectrum of Schrödinger operators on the whole space $\mathbf{R}^n$, see [17, 19]. For Schrödinger–type operators H on a bounded domain of $\mathbf{R}^n$ the spectral distribution function usually is asymptotical equivalent to a power function. For this case we give a simple sufficient condition for the admissibility of a thermodynamic equilibrium distribution function f in terms of the critical exponent of H, see Theorem 14. Birman and Solomyak calculate the critical exponent for a large class of self–adjoint elliptic differential operators, see Section 6, which allows to use our criterion for these operators H.

A straightforward application of our result is to the Euler equations of density functional theory *without* local density approximation of the exchange–correlation operator. Indeed, the existence and conditional uniqueness of solutions for these equations depends only on the monotonicity property of the density but it is not necessary that the exchange–correlation operator is a function, see [14, 15].

2 Preliminaries

Let $\mathfrak{H}$ be a separable Hilbert space with the scalar product $\langle \cdot, \cdot \rangle_{\mathfrak{H}}$. We use the following notations: $\mathcal{B}$, $\mathcal{B}_1$, and $\mathcal{B}_2$ are the spaces of bounded, trace class, and Schmidt class operators on $\mathfrak{H}$, respectively; $\mathcal{B}^{\mathfrak{s}}$, $\mathcal{B}_1^{\mathfrak{s}}$, and $\mathcal{B}_2^{\mathfrak{s}}$ are the subspaces of self–adjoint operators from $\mathcal{B}$, $\mathcal{B}_1$, and $\mathcal{B}_2$, respectively. We denote the scalars and the scalar multiples of the identity in $\mathcal{B}$ by the same symbol. For the dual pairing between $\mathcal{B}^*$ and $\mathcal{B}$ we write $\langle \cdot, \cdot \rangle$. Since ${\mathcal{B}_1}^* = \mathcal{B}$ there is $\mathcal{B}_1 \subseteq \mathcal{B}^*$; if $T \in \mathcal{B}_1$ and $S \in \mathcal{B}$, then $\langle T, S \rangle = \operatorname{tr}(TS)$, where $\operatorname{tr}(\cdot)$ denotes the trace.

Definition 1. *A mapping A on the domain space $\mathcal{B}$ into a Banach space X is sequentially w-continuous, if the convergence of a sequence $\{U_n\}_{n\in\mathbf{N}} \subset \mathcal{B}$ to $U \in \mathcal{B}$ in the weak operator topology ($\operatorname{w-lim}_{n\to\infty} U_n = U$) implies*

$$\lim_{n\to\infty} \|A(U_n) - A(U)\|_X = 0.$$

Remark 2. *In general the sequential w-continuity of A does not imply the continuity of A as a map from the topological vector space $\mathcal{B}$ endowed with the weak operator topology into X. However, any closed ball*

$$M_r(U) \stackrel{\text{def}}{=} \{V \in \mathcal{B} : \|U - V\|_{\mathcal{B}} \le r\}, \qquad r \in [0, \infty), \quad U \in \mathcal{B}$$

in $\mathcal{B}$ endowed with the weak operator topology is a compact, metrisable space and its topology possesses a countable base, see [8, 3.1]. Moreover, $M_r(U)$ is totally bounded, a fortiori bounded. As $M_r(U)$ is metrisable, $A : M_r(U) \to X$ is sequentially continuous if and only if it is topologically continuous, see [26, A6], if and only if the restriction of A to the space $M_r(U)$ is uniformly continuous. Furthermore, a set of operators from $\mathcal{B}$ is bounded in norm if and only if it is bounded in the weak operator topology. Hence, if A is a sequentially w-continuous mapping from $\mathcal{B}$ into X, then A is a bounded mapping with respect to both the norm topology and the weak operator topology in $\mathcal{B}$.

Definition 3. *Let ω be an even Sobolev mollifier, e.g.*

$$\omega(x) \stackrel{\text{def}}{=} \begin{cases} c \exp\left(\frac{1}{x^2-1}\right) & \text{if } |x| < 1, \\ 0 & \text{elsewhere,} \end{cases} \qquad \text{and} \qquad \int_{\mathbf{R}} \omega(x)\,\mathrm{d}x = 1.$$

We define the mollification A_τ of a sequentially w-continuous operator A defined on $\mathcal{B}$ into a Banach space X by the Bochner–integral

$$A_\tau(U) \stackrel{\text{def}}{=} \frac{1}{\tau} \int_{-\tau}^{\tau} \omega\left(\tfrac{t}{\tau}\right) A(U - t)\,\mathrm{d}t, \quad U \in \mathcal{B}, \quad t \in \mathbf{R}, \quad \tau \in (0, 1]. \tag{1}$$

Remark 4. *Definition 3 is justified, since the sequential w-continuity of A implies the continuity of the mapping*

$$\mathbf{R} \ni t \longmapsto A(U + t) \in X \tag{2}$$

for all $U \in \mathcal{B}$. Hence, for each $U \in \mathcal{B}$ the function (2) is Bochner–integrable on the closed interval $[-1, 1]$, see [11, IV Theorem 1.9].

Lemma 5. *If $A : \mathcal{B} \to X$ is sequentially w-continuous, then*

$$\lim_{\tau \to 0} \|A_\tau(U) - A(U)\|_X = 0 \quad \textit{for all } U \in \mathcal{B}. \tag{3}$$

Proof. Let $U \in \mathcal{B}$ be arbitrarily given; the ball $M_1(U)$ contains all operators $U - t$ with $|t| \le 1$. Hence, see Remark 2, for each $\epsilon > 0$ exists a $\delta \in (0, 1]$ such that $|t| < \delta$ yields $\|A(U - t) - A(U)\|_X < \epsilon$. Thus, for $\tau \in (0, \delta]$ one obtains

$$\|A_\tau(U) - A(U)\|_X \le \frac{1}{\tau} \int_{-\tau}^{\tau} \omega\big(\tfrac{t}{\tau}\big) \, \|A(U - t) - A(U)\|_X \, \mathrm{d}t < \epsilon.$$

□

Lemma 6. *If $A : \mathcal{B} \to X$ is sequentially w-continuous, then the maps A_τ, $\tau \in (0, 1]$, are sequentially w-continuous, uniformly in τ.*

Proof. If $\{U_n\}_{n \in \mathbf{N}}$ is a sequence in $\mathcal{B}$ with $\text{w-lim}_{n\to\infty} U_n = U$, then an $r > 0$ exists such that $U_n \in M_r(U)$ for all $n \in \mathbf{N}$. A is uniformly continuous on $M_{r+1}(U)$, endowed with the weak operator topology, see Remark 2. Hence, for each $\epsilon > 0$ elements $x_1, x_2, \ldots, x_k$, and $y_1, y_2, \ldots, y_k$ from $\mathfrak{H}$ exist such that

$$\sup_{j \in \{1,2,\ldots,k\}} |\langle (U_n - U)x_j, y_j \rangle_{\mathfrak{H}}| < 1 \tag{4}$$

yields

$$\|A(U_n - t) - A(U - t)\|_X < \epsilon \qquad \text{for all } t \in [-1, 1].$$

Thus, one obtains for all $\tau \in (0, 1]$ and all U_n which fulfil (4):

$$\|A_\tau(U_n) - A_\tau(U)\|_X \le \frac{1}{\tau} \int_{-\tau}^{\tau} \omega\big(\tfrac{t}{\tau}\big) \, \|A(U_n - t) - A(U - t)\|_X \, \mathrm{d}t < \epsilon.$$

□

Remark 7. *In particular, if $\mathfrak{H} = \mathbf{C} \cong \mathcal{B}$ and A is a continuous function on $\mathcal{B}^{\mathfrak{s}} = \mathbf{R}$, then A_τ is the usual mollification of A. Moreover, the functions A_τ, $\tau \in (0, 1]$, are continuous, uniformly in τ. If, additionally, $A : \mathbf{R} \to \mathbf{R}$ is bounded on $[0, \infty)$ and integrable on $[0, \infty)$, then the mollified functions A_τ, $\tau \in (0, 1]$, are bounded, integrable, and Lipschitz continuous—a fortiori Hölder continuous—on (a, ∞) for all $a \in \mathbf{R}$.*

Corollary 8. *If $A : \mathcal{B} \to X$ is sequentially w-continuous, then*

$$\lim_{\tau \to 0,\ n \to \infty} \|A(U) - A_\tau(U_n)\|_X = 0 \tag{5}$$

for all U, $U_n \in \mathcal{B}$ with $\text{w-lim}_{n\to\infty} U_n = U$.

Proof. Let $\epsilon > 0$ be given. We estimate

$$\|A(U) - A_\tau(U_n)\|_X \le \|A(U) - A_\tau(U)\|_X + \|A_\tau(U) - A_\tau(U_n)\|_X \, .$$

According to Lemmata 5 and 6 an $n_\epsilon \in \mathbf{N}$ and a $T \in (0, 1]$ exist such that the addends on the right hand side are smaller than $\epsilon/2$ for all $\tau \in (0, T)$ and all $n > n_\epsilon$.
□

3 Convexity and differentiability

In this section we state conditions on a function G such that the trace functional $\mathrm{tr}(G(H+U))$ is convex and differentiable with respect to the argument $U \in \mathcal{B}^{\mathfrak{s}}$; the gradient at U turns out to be $G'(H+U) \in \mathcal{B}_1$.

Assumption 9. *Throughout this paper H is a self–adjoint operator on a separable, infinite–dimensional Hilbert space $\mathfrak{H}$ which has a compact resolvent and is semi–bounded from below.*

Lemma 10. *Let G be a real valued, continuous function on $\mathbf{R}$ which is bounded on $[0,\infty)$. If the mapping*

$$A : \mathcal{B} \to \mathcal{B}, \qquad A(U) \stackrel{\text{def}}{=} G(H+U), \quad U \in \mathrm{dom}(A) = \mathcal{B}^{\mathfrak{s}} \tag{6}$$

is sequentially w-continuous, then

$$A_\tau(U) = G_\tau(H+U) \quad \text{for all } \tau \in (0,1] \text{ and all } U \in \mathcal{B}^{\mathfrak{s}}.$$

Proof. Under the preconditions of Lemma 10 the operators A and A_τ, $\tau \in (0,1]$, are well defined. If x and y are arbitrary elements from the Hilbert space $\mathfrak{H}$ and E_{H+U} is the spectral measure of the operator $H+U$, then

$$\begin{aligned}
\langle A_\tau(U)x, y\rangle_{\mathfrak{H}} &= \frac{1}{\tau}\int_{-\tau}^{\tau} \omega\left(\tfrac{t}{\tau}\right)\langle A(U-t)x, y\rangle_{\mathfrak{H}}\,\mathrm{d}t \\
&= \frac{1}{\tau}\int_{-\tau}^{\tau} \omega\left(\tfrac{t}{\tau}\right)\langle G(H+U-t)x, y\rangle_{\mathfrak{H}}\,\mathrm{d}t \\
&= \frac{1}{\tau}\int_{-\tau}^{\tau} \omega\left(\tfrac{t}{\tau}\right)\int_{-\infty}^{\infty} G(\lambda - t)\,\mathrm{d}\langle E_{H+U}(\lambda)x, y\rangle_{\mathfrak{H}}\,\mathrm{d}t \\
&= \int_{-\infty}^{\infty} \frac{1}{\tau}\left(\int_{-\tau}^{\tau} \omega\left(\tfrac{t}{\tau}\right) G(\lambda - t)\,\mathrm{d}t\right)\,\mathrm{d}\langle E_{H+U}(\lambda)x, y\rangle_{\mathfrak{H}} \\
&= \langle G_\tau(H+U)x, y\rangle_{\mathfrak{H}}.
\end{aligned}$$

□

Given an operator H according to Assumption 9, we introduce a class of functions G such that $\mathrm{tr}(G(H+U))$ is well defined for all $U \in \mathcal{B}^{\mathfrak{s}}$.

Definition 11. *Let $G : \mathbf{R} \to [0,\infty)$ be a continuous function and let H be according to Assumption 9. We say G belongs to the class $\mathfrak{F}_H$ if G is decreasing, i.e. if $s < t$ implies $G(s) \geq G(t)$, and $G(H+\gamma) \in \mathcal{B}_1$ for each $\gamma \in \mathbf{R}$.*

Remark 12. *$G \in \mathfrak{F}_H$ implies $\lim_{t\to\infty} G(t) = 0$. If, additionally, G is absolutely continuous, then $-G'$ is non–negative (because G is decreasing) and $G(t) = -\int_t^\infty G'(s)\,\mathrm{d}s$.*

The trace class condition on $G(H+\gamma)$ can be expressed in terms of the spectral distribution function (counting function)

$$\xi_H : \mathbf{R} \to \mathbf{N}, \qquad \xi_H(t) \overset{\text{def}}{=} \operatorname{tr}(E_H(t)) = \operatorname{tr}(E_H((-\infty,t)) =, \quad t \in \mathbf{R}, \tag{7}$$

where E_H is the spectral measure of H. $\xi_H(t)$ is the number of eigenvalues (including multiplicity) on the open interval $(-\infty, t)$.

Theorem 13. *Let $G : \mathbf{R} \to [0,\infty)$ be an absolutely continuous, decreasing function. The function G belongs to $\mathfrak{F}_H$ if and only if*

$$\sup_{\lambda \in [0,\infty)} \xi_H(\lambda-\gamma)G(\lambda) - \int_0^\infty \xi_H(\lambda-\gamma)G'(\lambda)\,\mathrm{d}\lambda < \infty. \tag{8}$$

for each $\gamma \in \mathbf{R}$.

Proof. It suffices to demonstrate for each $\gamma \in \mathbf{R}$: $G(H+\gamma) \in \mathcal{B}_1$ if and only if (8) holds. $G(H+\gamma) \in \mathcal{B}_1$ implies for all $t \in \mathbf{R}$:

$$\begin{aligned}
\operatorname{tr}(G(H+\gamma)) &= \int_{-\infty}^{\infty} G(\lambda+\gamma)\,\mathrm{d}\xi_H(\lambda) \\
&\geq \int_{-\infty}^{t-\gamma} G(\lambda+\gamma)\,\mathrm{d}\xi_H(\lambda) \\
&= G(t)\,\xi_H(t-\gamma) - \int_{-\infty}^{t} G'(\lambda)\,\xi_H(\lambda-\gamma)\,\mathrm{d}\lambda \\
&\geq G(t)\,\xi_H(t-\gamma) - \int_{0}^{t} G'(\lambda)\,\xi_H(\lambda-\gamma)\,\mathrm{d}\lambda;
\end{aligned}$$

it should be noted that both ξ_H and $-G'$ are non–negative functions, the latter one because G is decreasing. Passing now to the supremum over all $t \in [0,\infty)$ we get (8). Conversely, since H is semi–bounded from below (8) implies

$$\begin{aligned}
\infty &> \sup_{t \in [-\gamma,\infty)} \left(G(t+\gamma)\xi_H(t) - \int_{-\infty}^{t} G'(\lambda+\gamma)\xi_H(\lambda)\,\mathrm{d}\lambda \right) \\
&= \sup_{t \in [-\gamma,\infty)} \int_{-\infty}^{t} G(\lambda+\gamma)\,\mathrm{d}\xi_H(\lambda) \\
&= \int_{-\infty}^{\infty} G(\lambda+\gamma)\,\mathrm{d}\xi_H(\lambda) \\
&= \operatorname{tr}(G(H+\gamma)).
\end{aligned}$$

□

We give a necessary and sufficient criterion for G to belong to the class $\mathfrak{F}_H$ for the case that the spectral distribution function ξ_H of the operator H is asymptotically equivalent to some power function.

Theorem 14. *Let the spectral distribution function (7) of the operator H be such that*

$$0 < \lim_{\lambda \to \infty} \lambda^{-\theta} \xi_H(\lambda) < \infty \tag{9}$$

for some exponent $\theta > 0$. A decreasing, absolutely continuous function $G : \mathbf{R} \to [0, \infty)$ belongs to the class $\mathfrak{F}_H$ if and only if

$$-\int_0^\infty \lambda^\theta G'(\lambda)\,\mathrm{d}\lambda < \infty. \tag{10}$$

Proof. The proof rests on Theorem 13; first we prove that (10) implies $G \in \mathfrak{F}_H$. Let us define $g \stackrel{\text{def}}{=} -G'$; there is $g \geq 0$. We estimate the second addend in (8) for an arbitrary $\gamma \in \mathbf{R}$:

$$\begin{aligned} \int_{1+|\gamma|}^\infty \xi_H(\lambda-\gamma) g(\lambda)\,\mathrm{d}\lambda &\leq \sup_{\lambda \geq 1+|\gamma|} (\lambda-\gamma)^{-\theta} \xi_H(\lambda-\gamma) \int_{1+|\gamma|}^\infty (\lambda-\gamma)^\theta g(\lambda)\,\mathrm{d}\lambda \\ &\leq \sup_{\lambda \geq 1} \lambda^{-\theta} \xi_H(\lambda) \int_{1+|\gamma|}^\infty (\lambda-\gamma)^\theta g(\lambda)\,\mathrm{d}\lambda. \end{aligned}$$

If $\lambda \geq 1 + |\gamma|$, then $(\lambda-\gamma)^\theta \leq (\lambda + |\gamma|)^\theta \leq 2^\theta \lambda^\theta$; thus:

$$\int_{1+|\gamma|}^\infty \xi_H(\lambda-\gamma) g(\lambda)\,\mathrm{d}\lambda \leq 2^\theta \sup_{\lambda \geq 1} \lambda^{-\theta} \xi_H(\lambda) \int_0^\infty \lambda^\theta g(\lambda)\,\mathrm{d}\lambda$$

which yields

$$\int_0^\infty \xi_H(\lambda-\gamma) g(\lambda)\,\mathrm{d}\lambda < \infty. \tag{11}$$

As for the first addend in (8) we note that for all $\lambda \in [0, \infty)$:

$$\begin{aligned} G(\lambda) = \int_\lambda^\infty g(s)\,\mathrm{d}s = \int_\lambda^\infty s^{-\theta} s^\theta g(s)\,\mathrm{d}s & \\ &\leq \lambda^{-\theta} \int_\lambda^\infty s^\theta g(s)\,\mathrm{d}s \leq \lambda^{-\theta} \int_0^\infty s^\theta g(s)\,\mathrm{d}s. \end{aligned}$$

Hence, taking into account the precondition (10):

$$\sup_{\lambda \geq 0} \lambda^\theta G(\lambda) \leq \int_0^\infty s^\theta g(s)\,\mathrm{d}s < \infty.$$

Now we get

$$\begin{aligned} \sup_{\lambda \geq 1+|\gamma|} \xi_H(\lambda-\gamma) G(\lambda) &\leq \sup_{\lambda \geq 1+|\gamma|} (\lambda-\gamma)^{-\theta} \xi_H(\lambda-\gamma) \sup_{\lambda \geq 1+|\gamma|} (\lambda-\gamma)^\theta G(\lambda) \\ &\leq 2^\theta \sup_{\lambda \geq 1} \lambda^{-\theta} \xi_H(\lambda) \sup_{\lambda \geq 1} \lambda^\theta G(\lambda) \\ &\leq 2^\theta \sup_{\lambda \geq 1} \lambda^{-\theta} \xi_H(\lambda) \int_0^\infty s^\theta g(s)\,\mathrm{d}s, \end{aligned}$$

which yields according to (9) and (10):

$$\sup_{\lambda\geq 0}\xi_H(\lambda-\gamma)G(\lambda)<\infty. \tag{12}$$

(12) and (11) imply (8), thus by Theorem 13 G belongs to $\mathfrak{F}_H$.

Due to (9) constants $c>0$ and $\lambda_0\in\mathbf{R}$ exist, such that

$$c\,\lambda^\theta\leq\xi_H(\lambda)\qquad\text{for all }\lambda\geq\lambda_0$$

If $G\in\mathfrak{F}_H$, then, according to Theorem 13

$$-\int_{\lambda_0}^\infty\lambda^\theta G'(s)\,\mathrm{d}s\leq-\frac{1}{c}\int_{\lambda_0}^\infty\xi_H(s)G'(s)\,\mathrm{d}s<\infty,$$

which implies (10). □

If $G\in\mathfrak{F}_H$, then

$$G(H-\|U\|_{\mathcal{B}})\geq G(H+U)\geq 0\quad\text{for all }U\in\mathcal{B}^{\mathfrak{s}}.$$

Hence, $G(H+U)\in\mathcal{B}_1$ and we can define the functional $\phi:\mathcal{B}^{\mathfrak{s}}\to\mathbf{R}$

$$\phi(U)\overset{\text{def}}{=}\operatorname{tr}(G(H+U)),\quad U\in\operatorname{dom}(\phi)\overset{\text{def}}{=}\mathcal{B}^{\mathfrak{s}},\quad G\in\mathfrak{F}_H. \tag{13}$$

Lemma 15. *If $G\in\mathfrak{F}_H$, then the mapping*

$$\mathcal{B}^{\mathfrak{s}}\ni U\longmapsto G(H+U)\in\mathcal{B}_1 \tag{14}$$

and the functional (13) are sequentially w-continuous.

Proof. Let $\{U_n\}_{n\in\mathbf{N}}$ be a sequence from $\mathcal{B}^{\mathfrak{s}}$ so that $\text{w-lim}_{n\to\infty}U_n=U$. We decompose

$$\begin{aligned}&(H+U_n-i)^{-1}-(H+U-i)^{-1}\\&\qquad=\left((H+U_n-i)^{-1}(U-U_n)+1\right)(H+U-i)^{-1}(U-U_n)(H+U-i)^{-1}.\end{aligned}$$

$\text{w-lim}_{n\to\infty}U_n=U$ implies, as $(H+U-i)^{-1}$ is compact, $(H+U-i)^{-1}(U-U_n)\to 0$ in the strong operator topology and $(H+U-i)^{-1}(U-U_n)(H+U-i)^{-1}\to 0$ in the uniform operator topology. The sequence $\{U_n\}_{n\in\mathbf{N}}$ is bounded, let us say by r. Hence, $\{(H+U_n-i)^{-1}(U-U_n)+1\}_{n\in\mathbf{N}}$ is bounded in $\mathcal{B}$ and we obtain $H+U_n\to H+U$ in the norm resolvent sense. Thus, [25, Theorem VIII.20(a)] applies mutatis mutandis to $h\overset{\text{def}}{=}\sqrt{G}$ and the sequence $\{H+U_n\}_{n\in\mathbf{N}}$ and we get $h(H+U_n)\to h(H+U)$ in the uniform operator topology. Let $\lambda_j(U)$, $\lambda_j(U_n)$, $j\in\mathbf{N}$,

$n \in \mathbf{N}$, be the eigenvalues of $H+U$ and $H+U_n$, respectively, counting multiplicity. Since $H+U_n$ converges to $H+U$ in the norm resolvent sense one has

$$\lim_{n\to\infty} \lambda_j(U_n) = \lambda_j(U) \qquad \text{for all } j \in \mathbf{N},$$

see [16, IV §3.5], which yields, due to the continuity of G:

$$\lim_{n\to\infty} G\big(\lambda_j(U_n)\big) = G\big(\lambda_j(U)\big) \qquad \text{for all } j \in \mathbf{N}. \tag{15}$$

As $H+U_n \geq H-r$ there is $\lambda_j(U_n) \geq \lambda_j(-r)$, for all $j,n \in \mathbf{R}$. Due to the monotone decay of G we now get

$$G\big(\lambda_j(U_n)\big) \leq G\big(\lambda_j(-r)\big), \qquad \text{for all } j,n \in \mathbf{R}, \tag{16}$$

which implies

$$\operatorname{tr}\big(G(H+U_n)\big) = \sum_{j=1}^{\infty} G\big(\lambda_j(U_n)\big) \leq \sum_{j=1}^{\infty} G\big(\lambda_j(-r)\big) = \operatorname{tr}\big(G(H-r)\big) < \infty.$$

Using (15) and (16) one obtains

$$\lim_{n\to\infty} \operatorname{tr}\big(G(H+U_n)\big) = \operatorname{tr}\big(G(H+U)\big). \tag{17}$$

$G(H+U_n)$, $n \in \mathbf{N}$, and $G(H+U)$ are trace class operators, hence, $h(H+U_n) = \big(G(H+U_n)\big)^{1/2}$, $n \in \mathbf{N}$, and $h(H+U) = \big(G(H+U)\big)^{1/2}$ belong to the Schmidt class. Thus, we get from (17)

$$\lim_{n\to\infty} \big\|\big(G(H+U_n)\big)^{1/2}\big\|_{\mathcal{B}_2} = \big\|\big(G(H+U)\big)^{1/2}\big\|_{\mathcal{B}_2} \tag{18}$$

which yields

$$\sup_{n\in\mathbf{N}} \big\|\big(G(H+U_n)\big)^{1/2}\big\|_{\mathcal{B}_2} < \infty.$$

Thus, taking into account the weak compactness of the unit ball of $\mathcal{B}_2$, we find that $\big(G(H+U_n)\big)^{1/2}$ converges to $\big(G(H+U)\big)^{1/2}$ weakly in $\mathcal{B}_2$. Together with (18) this implies

$$\lim_{n\to\infty} \big\|\big(G(H+U_n)\big)^{1/2} - \big(G(H+U)\big)^{1/2}\big\|_{\mathcal{B}_2} = 0.$$

Finally, using the estimate

$$\begin{aligned}
&\big\|\big(G(H+U_n)\big) - \big(G(H+U)\big)\big\|_{\mathcal{B}_1} \\
&\qquad \leq \Big(\big\|\big(G(H+U_n)\big)^{1/2}\big\|_{\mathcal{B}_2} + \big\|\big(G(H+U)\big)^{1/2}\big\|_{\mathcal{B}_2}\Big) \\
&\qquad\qquad \times \big\|\big(G(H+U_n)\big)^{1/2} - \big(G(H+U)\big)^{1/2}\big\|_{\mathcal{B}_2}
\end{aligned}$$

one obtains the sequential w-continuity of (14), and hence, the sequential w-continuity of (13). □

Proposition 16. *(J. v. Neumann [20, chapter V.3]) If $G \in \mathfrak{F}_H$ is convex, then the functional (13) is convex.*

A comprehensive proof of Proposition 16 is given in [18]. — The convex, continuously differentiable functions from $\mathfrak{F}_H$ can be characterized as follows:

Lemma 17. *Let $G : \mathbf{R} \to [0, \infty)$ be continuously differentiable. G is convex and belongs to $\mathfrak{F}_H$ if and only if $G(H) \in \mathcal{B}_1$ and $-G' \in \mathfrak{F}_H$.*

Proof. Since G is a continuously differentiable, convex function $-G'$ is a continuous, decreasing function and

$$G(z) + (y - z)G'(z) \le G(y) \qquad \text{for all } y, z \in \mathbf{R}. \tag{19}$$

With $z = t + \gamma$ and $y = t + \gamma - 1$ one obtains due to the non–negativity of G:

$$-G'(t + \gamma) \le G(t + \gamma - 1) \qquad \text{for all } t, \gamma \in \mathbf{R}.$$

Therefore,

$$0 \le \operatorname{tr}\big(- G'(H + \gamma)\big) \le \operatorname{tr}\big(G(H + \gamma - 1)\big) = \big\|G(H + \gamma - 1)\big\|_{\mathcal{B}_1} < \infty$$

for all $\gamma \in \mathbf{R}$. Hence, $-G'(H + \gamma) \in \mathcal{B}_1$ for each $\gamma \in \mathbf{R}$, and thus, $-G' \in \mathfrak{F}_H$.

Conversely, if $-G' \in \mathfrak{F}_H$ then by definition $-G'$ is continuous, non–negative, and decreasing. Thus, G is decreasing, convex, and non–negative. The convexity of G implies by specifying $y = t$ and $z = t + \gamma$ in (19):

$$G(t + \gamma) \le G(t) + \gamma G'(t + \gamma), \qquad \text{for all } t, \gamma \in \mathbf{R}.$$

Therefore,

$$\begin{aligned} 0 \ \le\ \operatorname{tr}\big(G(H + \gamma)\big) &\ \le\ \operatorname{tr}\big(G(H)\big) + \gamma \operatorname{tr}\big(G'(H + \gamma)\big) \\ &\ \le\ \big\|G(H)\big\|_{\mathcal{B}_1} + \gamma\big\|G'(H + \gamma)\big\|_{\mathcal{B}_1} \ <\ \infty \end{aligned}$$

for all $\gamma \in \mathbf{R}$. Hence, $G(H + \gamma) \in \mathcal{B}_1$ for each $\gamma \in \mathbf{R}$, and thus, $G \in \mathfrak{F}_H$. □

Lemma 18. *If $G \in \mathfrak{F}_H$, then $G_\tau \in \mathfrak{F}_H$ for all $\tau > 0$.*

Proof. The assertion follows directly from Lemma 15, Remark 2, and the Definitions 11 and 3. Let G be from $\mathfrak{F}_H$. The mollified function is smooth. As G is non–negative and the mollifier ω is non–negative, G_τ is non–negative for all $\tau > 0$. G_τ is also decreasing: if $s < t$, then $G(s) \ge G(t)$, hence

$$G_\tau(s) = \frac{1}{\tau}\int_{-\tau}^{\tau} \omega\Big(\frac{\theta}{\tau}\Big) G(s - \theta)\, \mathrm{d}\theta \ge \frac{1}{\tau}\int_{-\tau}^{\tau} \omega\Big(\frac{\theta}{\tau}\Big) G(t - \theta)\, \mathrm{d}\theta = G_\tau(t).$$

Finally, according to Lemma 15 the map (14) is sequentially w-continuous. Hence, Definition 3, Remark 4 (there replacing X by $\mathcal{B}_1$) and Lemma 10 ensure $G_\tau(H+\gamma) \in \mathcal{B}_1$ for all $\gamma \in \mathbf{R}$. □

Lemma 19. *Let $G : \mathbf{R} \to \mathbf{R}$ be continuous; if G is bounded on $[0, \infty)$, then*

$$\|G_\tau(H + U)\|_{\mathcal{B}} \leq \sup_{\lambda(U)-1 \leq t < \infty} G(t) < \infty \quad \text{for all } U \in \mathcal{B}^{\mathfrak{s}},\ \tau \in (0, 1], \tag{20}$$

where $\lambda(U)$ is the smallest eigenvalue of the operator $H + U$.

Proof. The assertion follows directly from the precondition and (1); one estimates:

$$\|G_\tau(H + U)\|_{\mathcal{B}} \leq \sup_{\lambda(U) \leq t < \infty} G_\tau(t)$$
$$= \sup_{\lambda(U) \leq s < \infty} \frac{1}{\tau} \int_{-\tau}^{\tau} \omega\left(\tfrac{t}{\tau}\right) G(s - t)\, \mathrm{d}t \leq \sup_{\lambda(U)-\tau \leq t < \infty} G(t).$$

□

Proposition 20. *(see M. Sh. Birman and M. Z. Solomyak [3, Theorem 6.1 and Theorem 7.8]) Let G be a real–valued, continuously differentiable function on $\mathbf{R}$ such that for each $a \in \mathbf{R}$ the derivative G' is bounded, integrable, and Hölder continuous on (a, ∞). If $W \in \mathcal{B}_1^{\mathfrak{s}}$, then the function*

$$\mathbf{R} \ni s \longmapsto G(H + sW) \in \mathcal{B}_1$$

is continuously differentiable and

$$\frac{\mathrm{d}}{\mathrm{d}s} \operatorname{tr}\left(G(H + sW)\right)\Big|_{s=t} = \operatorname{tr}\left(G'(H + tW)W\right) \quad \text{for all } t \in \mathbf{R}. \tag{21}$$

Theorem 21. *Let $G \in \mathfrak{F}_H$ be continuously differentiable. If G' is bounded on $[0, \infty)$ and*

$$\mathcal{B}^{\mathfrak{s}} \ni U \longmapsto G'(H + U) \in \mathcal{B}_1 \quad \text{is sequentially } w\text{-continuous}, \tag{22}$$

then the functional (13) is Fréchet differentiable and its gradient

$$\partial\phi \ :\ \mathcal{B}^{\mathfrak{s}} \to \mathcal{B}_1^{\mathfrak{s}} \subseteq (\mathcal{B}^{\mathfrak{s}})^*$$

is given by

$$\partial\phi(U) = G'(H + U) \quad \text{for all } U \in \mathcal{B}^{\mathfrak{s}}. \tag{23}$$

Proof. According to Remark 12 the function G' is integrable on $[0, \infty)$. Let us first assume that G' is additionally Hölder continuous. Then, due to Proposition 20, the map $\Upsilon : \mathbf{R} \to \mathcal{B}_1$,

$$\Upsilon(s) \stackrel{\text{def}}{=} G(H + U + sW), \quad s \in \mathbf{R}, \quad U \in \mathcal{B}^{\mathfrak{s}}, \quad W \in \mathcal{B}_1^{\mathfrak{s}},$$

is continuously differentiable and there is for all $s \in \mathbf{R}$, $U \in \mathcal{B}^{\mathfrak{s}}$, and $W \in \mathcal{B}_1^{\mathfrak{s}}$:

$$\phi(U + sW) - \phi(U) = \int_0^s \operatorname{tr}(G'(H + U + tW)W)\, \mathrm{d}t. \tag{24}$$

If G' is not Hölder continuous we regard the mollified functions (1) of G. According to Lemma 6 and Lemma 18 each of the functions G_τ, $\tau \in (0,1]$, satisfies the preconditions of Theorem 21. Moreover, the functions G_τ are Hölder continuous, see Remark 7. Thus, (24) is valid for each G_τ, $\tau \in (0,1]$:

$$\phi_\tau(U+sW) - \phi_\tau(U) = \int_0^s \operatorname{tr}(G'_\tau(H+U+tW)W)\,\mathrm{d}t. \tag{25}$$

As for passing to the limit $\tau \to 0$ on the left hand side of (25): according to Lemma 15, the mapping (14) is sequentially w-continuous, hence, Lemma 5 (there replacing X by $\mathcal{B}_1$) applies to (14). In view of passing to the limit $\tau \to 0$ on the right hand side of (25) we note: the assertion of Lemma 5 holds for the mapping (22); the integrand

$$\operatorname{tr}\left(G'_\tau(H+U+tW)W\right) \le \|G'_\tau(H+U+tW)\|_{\mathcal{B}} \, \|W\|_{\mathcal{B}_1^{\mathfrak{s}}}$$

is uniformly bounded for all $\tau \in (0,1]$ and all $t \in [0,s]$, see Lemma 19. Hence, we can pass to the limit $\tau \to 0$ in (25) and get (24) for all G which are in agreement with the preconditions of Theorem 21.

If $W \in \mathcal{B}^{\mathfrak{s}}$, then there is a sequence of self–adjoint trace class operators $\{W_n\}_{n\in\mathbf{N}}$ such that $\text{w-lim}_{n\to\infty} W_n = W$. (24) applies to each W_n:

$$\phi(U+sW_n) - \phi(U) = \int_0^s \operatorname{tr}(G'(H+U+tW_n)W_n)\,\mathrm{d}t. \tag{26}$$

Passing in (26) to the limit $n \to \infty$, thereby observing (22), one obtains that the functional ϕ is Gâteaux differentiable and has the gradient (23).

According to (22) and (23), $\partial\phi$ is w-continuous. This implies that the functional (13) is not only Gâteaux but also Fréchet differentiable, see e.g. [28, Proposition 4.8(c)]. □

Remark 22. *If we tighten the preconditions of Theorem 21 such that G belongs to the Besov space $B^1_{\infty,1}$, then the proof becomes much easier using results by Peller [23, § 6], see also [5, Theorem 2.5], instead of Proposition 20.*

Theorem 23. *If $G \in \mathfrak{F}_H$ is continuously differentiable and convex, then the functional (13) is Fréchet differentiable and its gradient (23) is monotone.*

Proof. According to Lemma 17 there is $-G' \in \mathfrak{F}_H$. Hence, G' is bounded on $[0,\infty)$ and due to Lemma 15 one has (22). Thus, by Theorem 21 the functional (13) is Fréchet differentiable and has the gradient (23). According to Proposition 16, the functional ϕ is convex. This implies that its gradient $\partial\phi$ is monotone, see e.g. [11, chapter III Lemma 4.10]. □

Definition 24. *Let G be from $\mathfrak{F}_H$. By means of the functional (13) related to G we define the functions $\Gamma_U : \mathbf{R} \to \mathbf{R}$, $U \in \mathcal{B}^{\mathfrak{s}}$:*

$$\Gamma_U(t) \stackrel{\text{def}}{=} \phi(U-t) = \operatorname{tr}(G(H+U-t)), \qquad U \in \mathcal{B}^{\mathfrak{s}}, \quad t \in \mathbf{R}. \tag{27}$$

Lemma 25. *Let G be from $\mathfrak{F}_H$ and let Γ_U be according to Definition 24. For any $U \in \mathcal{B}^{\mathfrak{s}}$:*

1. *the function Γ_U is non–negative and continuous;*
2. *if G is convex, then Γ_U is convex;*
3. *if G is continuously differentiable and convex, then the function Γ_U is differentiable and*
$$\Gamma_U'(t) = -\operatorname{tr}\big(\partial\phi(U-t)\big) = -\operatorname{tr}\big(G'(H+U-t)\big), \quad t \in \mathbf{R}; \tag{28}$$
4. *if G is strictly decreasing, then Γ_U is strictly increasing and*
$$\lim_{t\to\infty} \Gamma_U(t) = \infty \quad \text{and} \quad \lim_{t\to-\infty} \Gamma_U(t) = 0. \tag{29}$$

Proof. The non–negativity of G implies directly the non–negativity of Γ_U and the continuity of Γ_U follows from Lemma 15. If G is convex, then Proposition 16 ensures the convexity of Γ_U. One obtains the differentiability of Γ_U and (28) by means of the chain rule from Theorem 23. As for the monotonicity and asymptotics of Γ_U: if $U \in \mathcal{B}^{\mathfrak{s}}$, then $H+U$ has a compact resolvent; let $\lambda_j(U)$, $j \in \mathbf{N}$, be the eigenvalues of $H+U$ counting multiplicity. Since, according to the preconditions, G is non–negative and strictly decreasing, $t_1 < t_2$ implies

$$0 < G(\lambda_j(U) - t_1) < G(\lambda_j(U) - t_2) \qquad \text{for all } j \in \mathbf{N}.$$

Hence, $\Gamma_U(t_1) < \Gamma_U(t_2)$ for $t_1 < t_2$. To get the first assertion in (29) we estimate

$$\lim_{t\to\infty} \sum_{j\in\mathbf{N}} G(\lambda_j - t) = \lim_{l\to\infty} \sum_{j\in\mathbf{N}} G(\lambda_j - \lambda_l) \geq \lim_{l\to\infty} l\, G(0) = \infty.$$

The second assertion in formula (29) follows from the majorant criterion, due to the convergence of $\sum_{j\in\mathbf{N}} G(\lambda_j)$. Consequently

$$\lim_{t\to-\infty} \sum_{j\in\mathbf{N}} G(\lambda_j - t) = \sum_{j\in\mathbf{N}} \lim_{t\to-\infty} G(\lambda_j - t) = 0,$$

see also Remark 12. ☐

Lemma 26. *Let Γ_U be according to Definition 24. If V, $W \in \mathcal{B}^{\mathfrak{s}}$ and $V \leq W$, then $\Gamma_V(t) \geq \Gamma_W(t)$ for all $t \in \mathbf{R}$.*

Proof. Let $\lambda_j(U)$, $j \in \mathbf{N}$, be the eigenvalues of $H+U$, $U \in \mathcal{B}^{\mathfrak{s}}$, counting multiplicity. If $V \leq W$, then the maximum principle implies $\lambda_j(V-t) \leq \lambda_j(W-t)$ for all $t \in \mathbf{R}$. Hence, $\Gamma_V(t) \geq \Gamma_W(t)$ for all $t \in \mathbf{R}$. ☐

4 Statistical operators

In the conceptual framework of quantum mechanics $H+U$ is a Hamiltonian with a kinetic energy part H and a potential energy part U. Let f be a strictly decreasing thermodynamic equilibrium distribution function for the quantum system under consideration. We define a generalized Fermi level $\varepsilon(U)$ such that $f(H+U-\varepsilon(U))$ is a statistical operator, that is a density matrix, see e.g. [20, IV.1]. This statistical operator is anti–monotone and continuous with respect to the argument U.

Definition 27. *We define the functional* $\mathcal{G} : \mathcal{B}^{\mathfrak{s}} \times \mathbf{R} \to \mathbf{R}$,

$$\mathcal{G}(U,t) \stackrel{\text{def}}{=} 1 - \operatorname{tr}(f(H+U-t)), \quad U \in \mathcal{B}^{\mathfrak{s}}, \quad t \in \mathbf{R}, \tag{30}$$

where $f \in \mathfrak{F}_H$ *is assumed to be strictly decreasing.*

Due to Lemma 25 (there replacing G by f) the functional (30) is well defined and

$$\text{if } \operatorname*{w-lim}_{n\to\infty} U_n = U \text{ and } \lim_{n\to\infty} t_n = t, \text{ then } \lim_{n\to\infty} \mathcal{G}(U_n,t_n) = \mathcal{G}(U,t), \tag{31}$$

$$\text{if} \quad t_1 < t_2, \quad \text{then} \quad \mathcal{G}(U,t_1) > \mathcal{G}(U,t_2) \qquad \text{for all } U \in \mathcal{B}^{\mathfrak{s}}, \tag{32}$$

$$\lim_{t\to\infty} \mathcal{G}(U,t) = -\infty \text{ and } \lim_{t\to-\infty} \mathcal{G}(U,t) = 1 \qquad \text{for all } U \in \mathcal{B}^{\mathfrak{s}}. \tag{33}$$

Theorem 28. *If* $f \in \mathfrak{F}_H$ *is strictly decreasing, then for any* $U \in \mathcal{B}^{\mathfrak{s}}$ *the equation* $\mathcal{G}(U,t) = 0$ *has a unique solution* $t = \varepsilon(U)$. *The functional* $\varepsilon : \mathcal{B}^{\mathfrak{s}} \to \mathbf{R}$ *is increasing, i.e. if* $V \le W$, *then* $\varepsilon(V) \le \varepsilon(W)$. *Moreover,* $\varepsilon : \mathcal{B}^{\mathfrak{s}} \to \mathbf{R}$ *is sequentially w-continuous, i.e.* $\operatorname{w-lim}_{n\to\infty} U_n = U$ *implies* $\lim_{n\to\infty} \varepsilon(U_n) = \varepsilon(U)$.

Proof. For any fixed $U \in \mathcal{B}^{\mathfrak{s}}$ the function $\mathbf{R} \ni t \mapsto \mathcal{G}(U,t)$ is continuous and strictly decreasing, see (31), (32). This implies in conjunction with (33) that the equation $\mathcal{G}(U,t) = 0$ has a unique solution for any $U \in \mathcal{B}^{\mathfrak{s}}$.

If $V \le W$, then Lemma 26 (there replacing G by f) implies

$$0 = \mathcal{G}(V, \varepsilon(V)) \le \mathcal{G}(W, \varepsilon(V)).$$

This yields $\varepsilon(V) \le \varepsilon(W)$, due to (32).

Now, let $\{U_n\}_{n\in\mathbf{N}} \subset \mathcal{B}^{\mathfrak{s}}$ be a sequence with $\operatorname{w-lim}_{n\to\infty} U_n = U$. Then $\{U_n\}_{n\in\mathbf{N}}$ is bounded in $\mathcal{B}$, let us say by r. This yields $-r \le U_n \le r$, hence,

$$\varepsilon(-r) \le \varepsilon(U_n) \le \varepsilon(r) \qquad \text{for all } n \in \mathbf{N},$$

thence $\{\varepsilon(U_n)\}_{n\in\mathbf{N}}$ is precompact. Let us assume there were a subsequence $\{U_{n_k}\}_{k\in\mathbf{N}}$ such that

$$\lim_{k\to\infty} \varepsilon(U_{n_k}) = t \ne \varepsilon(U).$$

Then (31) implies

$$\mathcal{G}(U, \varepsilon(U)) = 0 = \mathcal{G}(U_{n_k}, \varepsilon(U_{n_k})) = \mathcal{G}(U,t).$$

Hence, $\varepsilon(U) = t$. $\square$

Definition 29. *A function $f \in \mathfrak{F}_H$, see Definition 11, is said to belong to the class $\mathfrak{E}_H \subset \mathfrak{F}_H$, if it is strictly decreasing, and $F(H) \in \mathcal{B}_1^{\mathfrak{s}}$, where*

$$F(t) \stackrel{\mathrm{def}}{=} \int_t^\infty f(s)\,\mathrm{d}s.$$

For $f \in \mathfrak{E}_H$, the functional $\varepsilon : \mathcal{B}^{\mathfrak{s}} \to \mathbf{R}$ defined by the unique solution of the equation $\mathcal{G}(U, \varepsilon(U)) = 0$ is called the (generalized) Fermi level. Moreover, the functional $\Phi : \mathcal{B}^{\mathfrak{s}} \to \mathbf{R}$,

$$\Phi(U) \stackrel{\mathrm{def}}{=} \mathrm{tr}(F(H + U - \varepsilon(U)) - \varepsilon(U) = \phi(U - \varepsilon(U)) - \varepsilon(U) \tag{34}$$

is well defined, where ϕ is the functional (13) with respect to the function F.

Remark 30. *Theorem 28 ensures the existence of the Fermi level $\varepsilon(U)$. $f \in \mathfrak{E}_H$ if and only if f is the negative derivative of a function $F \in \mathfrak{F}_H$ which is continuously differentiable and strictly convex, see Lemma 17. If f is a strictly decreasing function in agreement with the preconditions of Theorem 14, then $f \in \mathfrak{E}_H$.*

Theorem 31. *If $f \in \mathfrak{E}_H$, then Φ from Definition 29 is convex.*

Proof. Since f is decreasing the function $F(t) \stackrel{\mathrm{def}}{=} \int_t^\infty f(s)\,\mathrm{d}s$ is convex. Thus, according to Lemma 25 (there replacing G by F), for any $U \in \mathcal{B}^{\mathfrak{s}}$ the function Γ_U, referring to $G = F$, is convex and differentiable, hence

$$\Gamma_U(z) + (y - z)\Gamma_U'(z) \le \Gamma_U(y), \quad y, z \in \mathbf{R}, \quad U \in \mathcal{B}^{\mathfrak{s}}. \tag{35}$$

Let V, W be from $\mathcal{B}^{\mathfrak{s}}$ and let t be from the interval $[0, 1]$. Inserting

$$U = tW + (1-t)V, \quad z = \varepsilon(tW + (1-t)V), \quad y = \varepsilon(W) + (1-t)\varepsilon(V)$$

into (35), thereby observing (28) and the implicit definition $\mathrm{tr}\big(f(H + U - \varepsilon(U))\big) = 1$ of the Fermi level, one obtains

$$\begin{aligned}\mathrm{tr}\,&\Big(F\big(H + tW + (1-t)V - t\varepsilon(W) - (1-t)\varepsilon(V)\big)\Big)\\ &\ge \mathrm{tr}\,\Big(F\big(H + tW + (1-t)V - \varepsilon(tW + (1-t)V)\big)\Big)\\ &\qquad + t\varepsilon(W) + (1-t)\varepsilon(V) - \varepsilon(tW + (1-t)V),\end{aligned}$$

or in terms of the functional (13) (there replacing G by F) and (34)

$$\begin{aligned}&\Phi\big(tW + (1-t)V\big)\\ &\quad\le \phi\Big(t\big(W - \varepsilon(W)\big) + (1-t)\big(V - \varepsilon(V)\big)\Big) - t\varepsilon(W) - (1-t)\varepsilon(V).\end{aligned}$$

Now, the convexity of ϕ, see Proposition 16, provides the assertion. □

Theorem 32. *Let $f \in \mathfrak{E}_H$ be continuously differentiable and let f' be bounded on $[0,\infty)$. If the map*

$$\mathcal{B}^{\mathfrak{s}} \ni U \longmapsto f'(H+U) \in \mathcal{B}_1^{\mathfrak{s}} \qquad \textit{is sequentially } w\textit{-continuous,} \tag{36}$$

then the Fermi level ε is Fréchet differentiable and its gradient is given by

$$\partial\varepsilon(U) = \frac{f'(H+U-\varepsilon(U))}{\operatorname{tr}(f'(H+U-\varepsilon(U))} \in \mathcal{B}_1^{\mathfrak{s}} \subset (\mathcal{B}^{\mathfrak{s}})^* \quad \textit{for all } U \in \mathcal{B}^{\mathfrak{s}}; \tag{37}$$

$\partial\varepsilon : \mathcal{B}^{\mathfrak{s}} \to \mathcal{B}_1^{\mathfrak{s}}$ is sequentially w-continuous.

Proof. According to Theorem 21 (there replacing G by f) the functional (30) has continuous partial derivatives

$$\partial_1\mathcal{G}(U,t) \in \mathcal{B}_1^{\mathfrak{s}} \subset (\mathcal{B}^{\mathfrak{s}})^*, \qquad \partial_2\mathcal{G}(U,t) \in \mathbf{R}^* \cong \mathbf{R}$$

on $\mathcal{B}^{\mathfrak{s}} \times \mathbf{R}$ which are given by

$$\begin{aligned} \langle \partial_1\mathcal{G}(U,t), W\rangle &= -\operatorname{tr}\big(f'(H+U-t)W\big), \\ \partial_2\mathcal{G}(U,t) &= \operatorname{tr}\big(f'(H+U-t)\big). \end{aligned}$$

Since f' is negative, $\partial_2\mathcal{G}(U,t) < 0$ for all $U \in \mathcal{B}^{\mathfrak{s}}$ and $t \in \mathbf{R}$. Thus, by the Implicit Function Theorem, for every $U \in \mathcal{B}^{\mathfrak{s}}$ there is a neighbourhood $\mathcal{U} \subset \mathcal{B}^{\mathfrak{s}}$ of U and a Fréchet differentiable function $\varepsilon : \mathcal{U} \to \mathbf{R}$ such that $\mathcal{G}(U,\varepsilon(U)) = 0$ for all $U \in \mathcal{U}$; the Fréchet derivative $\partial\varepsilon : \mathcal{U} \to (\mathcal{B}^{\mathfrak{s}})^*$ is given by (37) and it is sequentially w-continuous in $\mathcal{B}_1$. Finally, the nuclearity of $\partial\varepsilon(U)$ follows from the precondition (36). □

Theorem 33. *If $f \in \mathfrak{E}_H$, then the functional (34) is Fréchet differentiable, and*

$$\partial\Phi(U) = -f(H+U-\varepsilon(U)) \in \mathcal{B}_1^{\mathfrak{s}} \quad \textit{for all } U \in \mathcal{B}^{\mathfrak{s}}. \tag{38}$$

The mapping $\partial\Phi : \mathcal{B}^{\mathfrak{s}} \to \mathcal{B}_1^{\mathfrak{s}}$ is monotone and sequentially w-continuous.

Proof. Since f is decreasing the function $F(t) \stackrel{\text{def}}{=} \int_t^\infty f(s)\,\mathrm{d}s$ is convex and, according to Theorem 23, the functional (13) (there replacing G by F) is Fréchet differentiable. Let us first assume that f meets the preconditions of Theorem 32. Then the generalized Fermi level ε is Fréchet differentiable. Hence, the function $s \mapsto \Phi(U+sW)$, $s \in \mathbf{R}$, $U,W \in \mathcal{B}^{\mathfrak{s}}$ is differentiable in $s=0$ and

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}s}\Phi(U+sW)\Big|_{s=0} \\ &\qquad = \operatorname{tr}\left(\partial\phi\left(U-\varepsilon(U)\right)\left(W-\operatorname{tr}\left(\partial\varepsilon(U)W\right)\right)\right) - \operatorname{tr}\left(\partial\varepsilon(U)W\right) \\ &\qquad\qquad = -\operatorname{tr}\left(f(H+U-\varepsilon(U))W\right); \end{aligned}$$

thereby (23), (37), and $\operatorname{tr}\big(f(H+U-\varepsilon(U))\big)=1$ are taken into account. Hence, if f meets the preconditions of Theorem 32, the functional Φ is Gâteaux differentiable and has the gradient (38). Moreover, Lemma 15 and Theorem 28 assure the sequential w-continuity of $\partial\Phi$. Thus,

$$\Phi(U+sW)-\Phi(U)=-\int_0^s \operatorname{tr}(f(H+U+tW-\varepsilon(U+tW))W)\,\mathrm{d}t. \tag{39}$$

for all $s\in\mathbf{R}$, and U, $W\in\mathcal{B}^{\mathfrak{s}}$. Let us now assume $f\in\mathfrak{E}_H$. Then for each $\tau>0$ the mollified function f_τ meets the preconditions of Theorem 32, thus (39) applies to f_τ for each $\tau>0$. We pass to the limit $\tau\to0$. First we show

$$\lim_{\tau\to0}\varepsilon_\tau(U)=\varepsilon(U)\quad\text{for all } U\in\mathcal{B}^{\mathfrak{s}}. \tag{40}$$

According to the Definition 29 of the Fermi level ε_τ

$$\operatorname{tr}(f_\tau(H+U-\varepsilon_\tau(U)))=1 \qquad \text{for all } \tau>0,$$

or in terms of (30):

$$\begin{aligned} 0 &= 1-\frac{1}{\tau}\int_{-\tau}^{\tau}\omega\left(\frac{t}{\tau}\right)\operatorname{tr}\left(f(H+U-\varepsilon_\tau(U)-t)\right)\,\mathrm{d}t \\ &= \frac{1}{\tau}\int_{-\tau}^{\tau}\omega\left(\frac{t}{\tau}\right)\mathcal{G}(U,\varepsilon_\tau(U)+t)\,\mathrm{d}t, \quad \text{for all } \tau>0. \end{aligned}$$

As $t\mapsto\mathcal{G}(U,t)$ is strictly decreasing this implies

$$\mathcal{G}(U,\varepsilon_\tau(U)+\tau)<0<\mathcal{G}(U,\varepsilon_\tau(U)-\tau).$$

Hence,

$$\mathcal{G}(U-\tau,\varepsilon_\tau(U))<0=\mathcal{G}(U-\tau,\varepsilon(U-\tau))$$

and consequently

$$\varepsilon(U-\tau)<\varepsilon_\tau(U). \tag{41}$$

Analogously one obtains

$$\varepsilon(U+\tau)>\varepsilon_\tau(U). \tag{42}$$

Thus, observing the sequential w-continuity of the Fermi level,

$$\varepsilon(U)\le\liminf_{\tau\to0}\varepsilon_\tau(U)\le\limsup_{\tau\to0}\varepsilon_\tau(U)\le\varepsilon(U).$$

Next, we show

$$\lim_{\tau\to0}\Phi_\tau(U)=\Phi(U). \tag{43}$$

We estimate

$$|\Phi_\tau(U)-\Phi(U)|\le|\phi_\tau(U-\varepsilon_\tau(U))-\phi(U-\varepsilon(U))|+|\varepsilon_\tau(U)-\varepsilon(U)|\,.$$

Each term on the right hand side of this estimate tends to zero as $\tau \to 0$: for the last term this is true due to (40); for the first term Corollary 8 and (40) imply the assertion. Next, we show for all U, $W \in \mathcal{B}^{\mathfrak{s}}$:

$$\lim_{\tau \to 0} \operatorname{tr}\left(f_\tau(H + U - \varepsilon_\tau(U))\, W\right) = \operatorname{tr}\left(f(H + U - \varepsilon(U))\, W\right). \tag{44}$$

To that end we estimate

$$\begin{aligned} &\|f_\tau(H + U - \varepsilon_\tau(U)) - f(H + U - \varepsilon(U))\|_{\mathcal{B}_1} \\ &\qquad \leq \|f_\tau(H + U - \varepsilon_\tau(U)) - f_\tau(H + U - \varepsilon(U))\|_{\mathcal{B}_1} \\ &\qquad\qquad + \|f_\tau(H + U - \varepsilon(U)) - f(H + U - \varepsilon(U))\|_{\mathcal{B}_1}. \end{aligned}$$

According to Lemma 15, $f \in \mathfrak{F}_H$ implies the sequential w-continuity of the mapping

$$\mathcal{B}^{\mathfrak{s}} \ni U \mapsto f(H + U) \in \mathcal{B}_1.$$

Hence, Corollary 8 provides

$$\lim_{\tau \to 0} \|f(H + U - \varepsilon(U)) - f_\tau(H + U - \varepsilon_\tau(U))\|_{\mathcal{B}_1} = 0 \quad \text{for all } U \in \mathcal{B}^{\mathfrak{s}}$$

and a fortiori (44). According to (41), (42) and Theorem 28

$$\varepsilon(U - 1) < \varepsilon_\tau(U) < \varepsilon(U + 1) \qquad \text{for all } \tau \in (0, 1],$$

hence, for any V, $W \in \mathcal{B}^{\mathfrak{s}}$ the set

$$\{V + tW - \varepsilon_\tau(V + tW) \; : \; t \in [0, s], \tau \in (0, 1]\}$$

is bounded in $\mathcal{B}$. Thus, due to the sequential w-continuity of the mapping

$$\mathcal{B}^{\mathfrak{s}} \ni U \mapsto f(H + U - \varepsilon(U)) \in \mathcal{B}_1^{\mathfrak{s}},$$

for any V, $W \in \mathcal{B}^{\mathfrak{s}}$ a constant $c = c(V, W)$ exists such that

$$\begin{aligned} &\operatorname{tr}\left(f_\tau(H + V + tW - \varepsilon(V + tW))W\right) \\ &\qquad\qquad \leq \|f_\tau(H + V + tW - \varepsilon(V + tW))\|_{\mathcal{B}_1} \|W\|_{\mathcal{B}} < c \end{aligned}$$

for all $t \in [0, s]$, and all $\tau \in (0, 1]$, see Remark 2 and Lemma 6. Due to Lebesgue's dominated convergence theorem we obtain

$$\begin{aligned} &\lim_{\tau \to 0} \int_0^s \operatorname{tr}\left(f_\tau(H + U + tW - \varepsilon_\tau(U + tW))W\right) \mathrm{d}t \\ &\qquad\qquad = \int_0^s \operatorname{tr}\left(f(H + U + tW - \varepsilon(U + tW))W\right) \mathrm{d}t \end{aligned}$$

for all $s \in \mathbf{R}$ and all U, $W \in \mathcal{B}^{\mathfrak{s}}$. This in connection with (43) proves (39) for all $f \in \mathfrak{E}_H$.

The sequential w-continuity of $\partial\Phi$ is a consequence of Lemma 15 (there replacing G by f) and Theorem 28. The functional (34) is not only Gâteaux but also Fréchet differentiable because $\partial\Phi$ is sequentially w-continuous, see e.g. [28, Proposition 4.8(c)]. Finally, the monotonicity of the gradient $\partial\Phi$ follows from Theorem 31 and [11, Lemma 4.10, Ch. III]. $\square$

Remark 34. *Theorem 33 states, in particular, that $f(H+U-\varepsilon(U))$ is a statistical operator for any thermodynamic equilibrium distribution function f from $\mathfrak{E}_H$ and any $U \in \mathcal{B}^{\mathfrak{s}}$. Indeed, $f(H+U-\varepsilon(U))$ is non–negative, nuclear, and $\operatorname{tr}(f(H+U-\varepsilon(U))) = 1$. Hence, the mean value of an observable $W \in \mathcal{B}^{\mathfrak{s}}$ is given by $\operatorname{tr}(f(H+U-\varepsilon(U))\,W)$. If $W \in \mathcal{B}^{\mathfrak{s}}$ is a non–negative operator, then*

$$\operatorname{tr}(f(H+U-\varepsilon(U))\,W) = \operatorname{tr}\left(\sqrt{W}\,f(H+U-\varepsilon(U))\,\sqrt{W}\right) \geq 0$$

for all $U \in \mathcal{B}^{\mathfrak{s}}$.

5 Schrödinger operators

If f is a thermodynamic equilibrium distribution function for the quantum systems related to the Hamiltonians $H+U$, then the negative gradient (38) of the functional (34) is a density matrix for each $U \in \mathcal{B}^{\mathfrak{s}}$, see Remark 34. With regard to the real space representation of quantum mechanics we investigate the mapping $-\partial\Phi$ for the special case that $\mathfrak{H}$ is a space of square integrable functions and U is induced by an essentially bounded, real–valued function u. It turns out that the corresponding density matrices can be represented by the non–negative, integrable functions.

Let $\mathfrak{H} = L^2(\mu)$ be a space of square integrable, complex–valued functions on a σ–finite measure space $(Y, \mathfrak{S}, \mu)$; further, let $L^1(\mu)$ and $L^\infty(\mu)$ be the spaces of integrable and essentially bounded functions on $(Y, \mathfrak{S}, \mu)$. Each element u from the space $L^\infty(\mu)$ induces a bounded multiplication operator $\pi(u)$ on $L^2(\mu)$. In this sense $L^\infty(\mu)$ embeds into $\mathcal{B}$.

Lemma 35. *Let $(Y, \mathfrak{S}, \mu)$ be a σ–finite measure space. If*

$$\pi : L^1(\mu)^* \cong L^\infty(\mu) \longrightarrow \mathcal{B}$$

is the natural embedding, then the dual mapping

$$\pi^* : \mathcal{B}^* \longrightarrow L^\infty(\mu)^* \cong L^1(\mu)^{**}$$

has the following properties:

1. *the restriction of π^* to the sub-space $\mathcal{B}_1 \subset \mathcal{B}^*$ maps onto $L^1(\mu)$;*
2. *the restriction of π^* to the sub-space $\mathcal{B}_1^{\mathfrak{s}} \subset (\mathcal{B}^{\mathfrak{s}})^*$ maps onto $L^1_{\mathbf{R}}(\mu)$;*

3. *the restriction of π^* to the self–adjoint, non–negative trace-class operators maps onto the real–valued, non–negative functions from $L^1(\mu)$.*

Proof. First, we show that for a trace class operator K the functional

$$L^\infty(\mu) \ni u \longmapsto \operatorname{tr}(K\pi(u))$$

is not only from $L^\infty(\mu)^*$ but from the pre-dual $L^1(\mu)$ of $L^\infty(\mu)$. Any trace-class operator K is given by two Hilbert-Schmidt operators K_1, K_2 such that $K = K_1K_2$. Each of the Hilbert-Schmidt operators K_1, K_2 is an integral operator with kernel k_1, $k_2 \in L^2(\mu \times \mu)$, respectively. For every $u \in L^\infty(\mu)$ the function $k_0 \stackrel{\text{def}}{=} k_2(1 \otimes u)$ belongs to $L^2(\mu \times \mu)$. Thus, k_0 is the kernel of an integral operator K_0 which is a Hilbert-Schmidt operator. Hence, $K_1K_0 = K\pi(u)$ is a trace class operator and

$$\begin{aligned}\operatorname{tr}(K\pi(u)) = \operatorname{tr}(K_1K_0) = \int\int k_1(s,t)k_0(t,s)\,\mathrm{d}\mu(t)\,\mathrm{d}\mu(s) \\ = \int\int k_1(s,t)k_2(t,s)\,\mathrm{d}\mu(t)u(s)\,\mathrm{d}\mu(s).\end{aligned}$$

Therefore, the functional $\pi^*(K) \in L^\infty(\mu)^*$ is given by the integrable function

$$s \longmapsto \int k_1(s,t)k_2(t,s)\,\mathrm{d}\mu(t).$$

Hence, the restriction of the embedding operator π to the subspace $\mathcal{B}_1$ of $\mathcal{B}$ maps into $L^1(\mu)$. The range of $\pi^*|_{\mathcal{B}_1}$ is closed because

$$(\pi^*|_{\mathcal{B}_1})^* = \pi : L^1(\mu)^* = L^\infty(\mu) \longrightarrow {\mathcal{B}_1}^* = \mathcal{B}$$

and the range of π is closed in $\mathcal{B}$, see [26, Theorem 4.14]. Moreover, the range of $\pi^*|_{\mathcal{B}_1}$ is dense in $L^1(\mu)$, because $\pi = (\pi^*|_{\mathcal{B}_1})^*$ is injective, see [26, Theorem 4.12].

The second assertion can be proved by applying the above argument mutatis mutandis to the embedding operator $\pi|_{L^\infty_{\mathbf{R}}(\mu)} : L^\infty_{\mathbf{R}}(\mu) \to \mathcal{B}^{\mathfrak{s}}$.

Finally, π maps the non–negative cone of $L^\infty_{\mathbf{R}}$ into the non–negative cone of $\mathcal{B}^{\mathfrak{s}}$. Hence, π^* maps the non–negative cone of $\mathcal{B}^{\mathfrak{s}*}$ into the non–negative cone of $L^\infty_{\mathbf{R}}(\mu)^*$. Therefore, π^* maps the self–adjoint, non–negative trace-class operators onto the functions $u \in L^1_{\mathbf{R}}(\mu)$ for which $\int uv\,\mathrm{d}\mu \geq 0$ for all v from the non–negative cone of $L^\infty_{\mathbf{R}}$, that is just the non–negative cone of $L^1_{\mathbf{R}}(\mu)$. $\square$

Each element u from the space $L^\infty_{\mathbf{R}}(\mu)$ induces a self–adjoint, bounded multiplication operator $\pi(u)$ on $L^2(\mu)$. If f belongs to the class $\mathfrak{C}_H$ from Definition 29, then, according to Theorem 33, the functional (34) is Fréchet differentiable and its gradient at $\pi(u) \in \mathcal{B}^{\mathfrak{s}}$ is the trace class operator $\partial\Phi(\pi(u)) = -f(H + \pi(u) - \varepsilon(\pi(u)))$.

Theorem 36. *Let $(Y, \mathfrak{S}, \mu)$ be a σ–finite measure space. If $f \in \mathfrak{E}_H$, then the restriction of the mapping (38) to the space $L^\infty_{\mathbf{R}}(\mu)$ maps into the non–positive cone of the space $L^1_{\mathbf{R}}(\mu)$ and the mapping*

$$\pi^* \partial\Phi\pi : L^\infty_{\mathbf{R}}(\mu) \to L^1_{\mathbf{R}}(\mu)$$

is monotone and continuous.

Proof. If $u \in L^\infty_{\mathbf{R}}(\mu)$, then $\pi(u) \in \mathcal{B}^{\mathfrak{s}}$, thence $-\partial\Phi(\pi(u))$ is a non–negative, self–adjoint trace-class operator and, according to Lemma 35, $\pi^*(-\partial\Phi(\pi(u)))$ is a real–valued, non–negative μ-integrable function.

The second assertion follows from the monotonicity and sequential w-continuity of $\partial\Phi$, see Theorem 33, and the fact that the embedding operator $\pi : L^\infty \to \mathcal{B}$ is linear and continuous, see e.g. [11, III Lemma 1.4]. □

Corollary 37. *If a thermodynamic equilibrium distribution function f belongs to the class $\mathfrak{E}_H$, then the density*

$$\mathcal{N}(u) \stackrel{\text{def}}{=} -\pi^*(\partial\Phi(\pi(u))) = \pi^*(f(H + \pi(u) - \varepsilon(\pi(u)))), \quad u \in L^\infty_{\mathbf{R}}(\mu)$$

associated to f and the Hamiltonian $H + \pi(u)$ is non–negative and μ-integrable. The mapping $\mathcal{N} : L^\infty_{\mathbf{R}}(\mu) \to L^1_{\mathbf{R}}(\mu)$ is continuous and anti–monotone.

Remark 38. *For a wide range of thermodynamic equilibrium distribution functions f the mapping $\mathcal{N}$ can be continuously and anti–montone extended to potentials u from other summability classes than $L^\infty(\mu)$, for instance from $L^2(\mu)$. This is possible, in particular, if the functions from $L^2(\mu)$ (regarded as multiplication operators) are infinitesimally small with respect to H and f decays rapidly enough.*

6 Self–adjoint elliptic differential operators

For Schrödinger–type operators H on a bounded domain $\Omega \subset \mathbf{R}^n$, $n > 0$, the spectral distribution function usually is asymptotical equivalent to a power function, that means for some $\theta > 0$:

$$0 < \lim_{\lambda \to \infty} \lambda^{-\theta} \xi_H(\lambda) < \infty; \tag{45}$$

θ is the critical exponent of H. Theorem 14 states a sufficient condition on a thermodynamic equilibrium distribution function f in terms of the critical exponent of H such that Corollary 37 applies. Birman and Solomyak proved (45) for a large class of self–adjoint elliptic differential operators thereby explicitly calculating the critical exponent.

In the following we regard self–adjoint elliptic differential operators acting on functions defined on a bounded domain Ω of the $\mathbf{R}^n$ with values which are complex $k \times k$ matrices. We abbreviate $D_j \stackrel{\text{def}}{=} -\partial/\partial x_j$. If $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$ is a multi–index, then $|\sigma| \stackrel{\text{def}}{=} \sigma_1 + \sigma_2 + \ldots + \sigma_n$ and $D^\sigma \stackrel{\text{def}}{=} D_1^{\sigma_1} D_2^{\sigma_2} \ldots D_n^{\sigma_n}$.

Assumption 39. *Let $\Omega \subset \mathbf{R}^n$ be a bounded domain and let $a : \Omega \to \mathbf{C}^{\nu^2}$ be a matrix–valued measurable function, such that $a(x)$ is a block–matrix consisting of symmetric $k \times k$ matrices $a(x) = \{a_{\sigma\varsigma}\}_{|\sigma|=|\varsigma|=l}$, where σ and ς are multi–indices, $l \in \mathbf{N}$ is a given number, and ν is k times the number of multi–indices σ with $|\sigma| = l$. We assume that the matrix $a(x)$ is non—negative and invertible for almost every $x \in \Omega$ and*

$$\|a\|_{\mathbf{C}^{\nu^2}} \in L^1_{loc}(\Omega), \quad \|a^{-1}\|_{\mathbf{C}^{\nu^2}} \in L^\kappa(\Omega), \qquad \frac{1}{\kappa} < \frac{2l}{n}, \qquad 1 \le \kappa \le \infty. \tag{46}$$

Proposition 40. *([4]) Under Assumption 39 the sesquilinear form*

$$\mathfrak{h}[u,v] \overset{\text{def}}{=} \sum_{|\sigma|=|\varsigma|=l} \int_\Omega \langle a_{\sigma\varsigma}(x) D^\sigma u, D^\varsigma v\rangle_{\mathbf{C}^k} \, \mathrm{d}x, \quad u, v \in C_0^\infty(\Omega, \mathbf{C}^k) \tag{47}$$

is symmetric, positive, and closable in the Hilbert space $L^2(\Omega, \mathbf{C}^k)$. The closure of $\mathfrak{h}$ uniquely determines a self–adjoint, positive operator H on $L^2(\Omega, \mathbf{C}^k)$.

Proposition 41. *([4, Theorem 2]) Under Assumption 39 the critical exponent of the operator H from Proposition 40 is $n/(2l)$.*

The sesquilinear form $\mathfrak{h}$ can be perturbed by forms of lower order without changing the critical exponent of the associated operator.

Proposition 42. *([4, Theorem 2]) Let us assert Assumption 39 and let $2j$ be a non–negative integer such that $j < l$. Then the sesquilinear form*

$$\mathfrak{b}[u,v] \overset{\text{def}}{=} \sum_{\substack{|\sigma|+|\varsigma|=2j \\ |\sigma|\le l,\, |\varsigma| \le l}} \int_\Omega \langle b_{\sigma\varsigma}(x) D^\sigma u, D^\varsigma v\rangle_{\mathbf{C}^k} \, \mathrm{d}x, \quad u, v \in C_0^\infty(\Omega, \mathbf{C}^k) \tag{48}$$

is relatively compact with respect to $\mathfrak{h}$, if the coefficients $b_{\sigma\varsigma}$ are measurable functions with symmetric $k \times k$ matrix–values such that for all multi–indices σ, ς from the range of the sum in (48) holds:

$$b_{\sigma\varsigma} \in L^{\varkappa_{\sigma\varsigma}}(\Omega, \mathbf{C}^k), \qquad 1 < \varkappa_{\sigma\varsigma} \le \infty, \qquad \tfrac{1}{\kappa} + \tfrac{1}{\varkappa_{\sigma\varsigma}} < 2\,\tfrac{l-j}{n}$$
$$\tfrac{1}{\kappa} + \tfrac{2}{\varkappa_{\sigma\varsigma}} < 2\,\tfrac{l-|\sigma|}{n} + 1, \qquad \tfrac{1}{\kappa} + \tfrac{2}{\varkappa_{\sigma\varsigma}} < 2\,\tfrac{l-|\varsigma|}{n} + 1.$$

The sum $\mathfrak{h} + \mathfrak{b}$ of the forms (47) and (48) is semi–bounded from below and closable in $L^2(\Omega, \mathbf{C}^k)$. The critical exponent of the self–adjoint, semi–bounded (from below) operator associated to the closure of $\mathfrak{h} + \mathfrak{b}$ is the critical exponent of H, namely $n/(2l)$.

Proposition 43. *([4, Theorem 2]) Let us assert Assumption 39 and let $2j$ be a non–negative integer such that $j < l$. Then the sesquilinear form*

$$\mathfrak{b}[u,v] \overset{\text{def}}{=} \sum_{\substack{|\sigma|+|\varsigma|=2j \\ |\sigma|\le l,\, |\varsigma| \le l}} \int_\Omega \langle\, \mathrm{d}\mu_{\sigma\varsigma}(x) D^\sigma u, D^\varsigma v\rangle_{\mathbf{C}^k}\,, \quad u, v \in C_0^\infty(\Omega, \mathbf{C}^k) \tag{49}$$

is relatively compact with respect to $\mathfrak{h}$*, if the* $\mu_{\sigma\varsigma}$ *are symmetric* $k \times k$ *matrices of finite Borel measures such that for all multi–indices* σ*,* ς *from the range of the sum in (49) holds:*

$$\frac{1}{\kappa} < 2\frac{l-|\sigma|}{n} - 1, \qquad \frac{1}{\kappa} < 2\frac{l-|\varsigma|}{n} - 1.$$

The sum $\mathfrak{h} + \mathfrak{b}$ *of the forms (47) and (49) is semi–bounded from below and closable in* $L^2(\Omega, \mathbf{C}^k)$*. The critical exponent of the self–adjoint, semi–bounded (from below) operator associated to the closure of* $\mathfrak{h} + \mathfrak{b}$ *is the critical exponent of* H*, namely* $n/(2l)$*.*

Remark 44. *One can sum up perturbations (48) and (49) for* $j = 0, 1, \ldots, l-1$*. If Proposition 42 or Proposition 43 applies to each of the addends, then the assertion of these Propositions holds mutatis mutandis for the sum of the perturbations. — For results about the critical exponent of elliptic operators on manifolds see e.g. [1, 2].*

Proposition 41 comprises, inter alia, the kinetic energy part of Schrödinger operators, including one–electron Hamiltonians in effective mass approximation with piecewise continuous effective mass tensors. Proposition 42 provides for such Hamiltonians with an additional magnetic field term.

References

[1] M. S. Agranovich, *Elliptic operators on closed manifolds*, Partial Differential Equations VI, Encyclopaedia of Mathematical Sciences, vol. 63, Springer-Verlag, Berlin, 1994, pp. 1-130 (English. Russian original).

[2] ______, *Elliptic boundary problems*, Partial Differential Equations IX, Encyclopaedia of Mathematical Sciences, vol. 79, Springer-Verlag, Berlin, 1997, pp. 1-144 (English. Russian original).

[3] M. Sh. Birman and M. Z. Solomyak, *Double Stieltjes operator integrals. III*, Problems in Mathematical Physics, vol. 6, Izdat. Leningrad. Univ., 1973, pp. 27-53 (Russian).

[4] ______, *Spectral asymptotics of nonsmooth elliptic operators II*, Trudy Mosk. matem. obsh. **28** (1973), 3-34 (Russian).

[5] ______, *Operator integration, perturbations and commutators*, Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) **170** (1989), no. Issled. Linein. Oper. Teorii Funktsii. 17, 34-66, 321.

[6] Ph. Caussignac, B. Zimmermann, and R. Ferro, *Finite element approximation of electrostatic potential in one dimensional multilayer structures with quantized electronic charge*, Computing **45** (1990), 251-264.

[7] R. Dingle, *Confined carrier quantum states in ultrathin semiconductor heterostructures*, Festkörperprobleme **15** (1975), 21-48.

[8] J. Dixmier, *Von Neumann Algebras*, North-Holland Mathematical Library, vol. 27, North-Holland Publishing Company, Amsterdam, 1981.

[9] H. Gajewski, *On existence, uniqueness and asymptotic behavior of solutions of the basic equations for carrier transport in semiconductors*, Z. Angew. Math. Mech. **65** (1985), 101-108.

[10] ______, *Analysis und Numerik von Ladungstransport in Halbleitern (Analysis and numerics of carrier transport in semiconductors)*, Mitt. Ges. Angew. Math. Mech. **16** (1993), 35-57 (German).

[11] H. Gajewski, K. Gröger, and K. Zacharias, *Nichtlineare Operatorgleichungen und Operatordifferentialgleichungen (Nonlinear operator equations and operator differential equations)*, Akademie-Verlag, Berlin, 1974 (German).

[12] H.-Chr. Kaiser and J. Rehberg, *On stationary Schrödinger-Poisson equations*, Z. Angew. Math. Mech. **75** (1995), 467-468.

[13] ______, *On stationary Schrödinger-Poisson equations modelling an electron gas with reduced dimension*, Mathematical Methods in the Applied Sciences **20** (1997), 1283-1312.

[14] ______, *About a one-dimensional stationary Schrödinger-Poisson system with Kohn-Sham potential*, Zeitschrift für Angewandte Mathematik und Physik **50** (1999), 423-458.

[15] ______, *About a stationary Schrödinger-Poisson system with Kohn-Sham potential in a bounded two- or three-dimensional domain*, Nonlinear Anal. Theory Methods Appl. **41** (2000), 33-72.

[16] T. Kato, *Perturbation theory for linear operators*, Grundlehren der mathematischen Wissenschaften, vol. 132, Springer-Verlag, Berlin, 1984.

[17] V. Kondratiev, V. Maz'ya, and M. Shubin, *Discreteness of spectrum and positivity criteria for magnetic Schrödinger operators*, Tech. report, arXiv:math.SP/0206140 v4, 27 February 2003.

[18] E. Lieb and G. K. Pedersen, *Convex multi-variable trace functions*, Rev. Math. Phys. **14** (2002), 631-648.

[19] V. Maz'ya and M. Shubin, *Discreteness of spectrum and positivity criteria for Schrödinger operators*, Tech. report, arXiv:math.SP/0305278 v1, 19 May 2003.

[20] J. v. Neumann, *Mathematische Grundlagen der Quantenmechanik*, Grundlehren der mathematischen Wissenschaften, vol. 38, Springer-Verlag, Berlin, 1932 (German).

[21] F. Nier, *A Stationary Schrödinger-Poisson System Arising from the Modelling of Electronic Devices*, Forum Mathematicum **2** (1990), 489.

[22] ______, *A variational formulation of Schrödinger-Poisson systems in dimensions* $d \leq 3$, Commun. in Partial Differential Equations **18** (1993), 1125-1147.

[23] V. V. Peller, *Hankel operators in the perturbation theory of unitary and self-adjoint operators.*, Funct. Anal. Appl. **19** (1985), 111-123 (Russian, English).

[24] S. J. Polak, C. den Heuer, W. H. A. Schilders, and P. Markowich, *Semiconductor device modelling from the numerical point of view.*, Int. J. Numer. Methods Eng. **24** (1987), 763-838.

[25] M. Reed and B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis*, Academic Press, New York, 1973.

[26] W. Rudin, *Functional analysis*, McGraw-Hill, New York, 1973.

[27] C. Weisbuch and B. Vinter, *Quantum semiconductor structures: Fundamentals and applications*, Academic Press, Boston, 1991.

[28] E. Zeidler, *Nonlinear functional analysis and its applications. I: Fixed point theorems*, Springer-Verlag, Berlin, 1986.