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SOME TRACE MONOTONICITY PROPERTIES AND APPLICATIONS

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ABSTRACT. We present some results on the monotonicity of some traces involving functions of self-adjoint operators with respect to the natural ordering of their associated quadratic forms. The relation between these results and Löwner's Theorem is discussed. We also apply these results to complete a proof of the Wegner estimate for continuum models of random Schrödinger operators as given in a 1994 paper by Combes and Hislop.

1. Statement of the problem and result

We consider two lower-semibounded self-adjoint operators A and B associated with closed symmetric, lower-semibounded quadratic forms q_A and q_B with form domains Q(A) and Q(B), respectively. We suppose that $q_A \leq q_B$. This inequality means that $Q(B) \subset Q(A)$ and that, for all $\varphi \in Q(B)$, we have $q_A(\varphi) \leq q_B(\varphi)$. Under these conditions, Kato proved in [8, Theorem 2.21, chapter VI] the following relationship between the resolvents of the two operators A and B. For all $a > -\inf \sigma(A)$, we have

$$(B+a)^{-1} \le (A+a)^{-1}.$$
(1.1)

This resolvent inequality may be used to derive several interesting relations between the traces of functions of A and B under some additional assumptions. We will prove that if $f \ge 0$ and g is a member of a class of functions \mathcal{L} described

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in Definition 2.1, then

$$\operatorname{Tr}(f(B)g(B)) \leq \operatorname{Tr}(f(B)g(A))$$

(see Theorem 2.4). We compare these inequalities with Löwner's Theorem (see Section 3) on operator monotone functions. We also use these results to complete a proof of Wegner's estimate for random Schrödinger operators given in [4]. These results rely on the following technical theorem.

Theorem 1.1. Suppose that A and B are two lower semibounded self-adjoint operators with quadratic forms q_A and q_B and form domains Q(A) and Q(B). Suppose that A and B are relatively form bounded in that

- (1) the form domains satisfy $Q(B) \subset Q(A)$, and
- (2) for all $\psi \in Q(B)$, we have $q_A(\psi) \leq q_B(\psi)$.

Let P_B be an orthogonal projection onto a *B*-invariant subspace so that, for some $m \in \mathbb{N}$ and for all $a > -\inf \sigma(A)$, the operators $P_B(B+a)^{-m}$ and $P_B(A+a)^{-m}$ are in the trace class. Then we have

(1) for all $n \in \mathbb{N}$ large enough so that $m < 2^n$ and for all $a > -\inf \sigma(A)$,

$$\operatorname{Tr}(P_B(B+a)^{-2^n}) \le \operatorname{Tr}(P_B(A+a)^{-2^n});$$

(2) for any t > 0,

$$\operatorname{Tr}(P_B e^{-tB}) \leq \operatorname{Tr}(P_B e^{-tA}).$$

Proof. 1. We first note that, by the assumptions that $P_B(B+a)^{-m}$ and $P_B(A+a)^{-m}$ are trace class for some integer $m \geq 0$, it follows that the operators in statements (1) and (2) are all in the trace class since they may be expressed as products of an operator in the trace class and a bounded operator, such as $P_B e^{-tA} = P_B(A+a)^{-m} \cdot (A+a)^m e^{-tA}$. The result of Kato [8, Theorem 2.21, chapter VI], stated above, implies that $(B+a)^{-1} \leq (A+a)^{-1}$. We first suppose that P_B is a nonzero rank 1 projection $P_B = P_\lambda$, so that $BP_\lambda = \lambda P_\lambda$. From inequality (1.1), it follows that for $a > -\inf \sigma(A)$, we have

$$\operatorname{Tr} P_{\lambda} = (\lambda + a) \operatorname{Tr} \left(P_{\lambda} (B + a)^{-1} \right)$$

$$\leq (\lambda + a) \operatorname{Tr} \left(P_{\lambda} (A + a)^{-1} \right)$$

$$\leq (\lambda + a) \| P_{\lambda} \|_{2} \| P_{\lambda} (A + a)^{-1} \|_{2}.$$
(1.2)

Since P_{λ} is a rank 1 projector, we have

$$||P_{\lambda}||_{2} = ||P_{\lambda}||_{1} = \operatorname{Tr} P_{\lambda} = 1,$$
 (1.3)

and

$$||P_{\lambda}(A+a)^{-1}||_{2} = (\operatorname{Tr} P_{\lambda}(A+a)^{-2})^{1/2}.$$
 (1.4)

Upon squaring inequality (1.2) and using the results (1.3)-(1.4), we obtain

$$\operatorname{Tr} P_{\lambda} \leq (\lambda + a)^{2} \left\| P_{\lambda} (A + a)^{-1} \right\|_{2}^{2} \\ = (\lambda + a)^{2} \operatorname{Tr} \left(P_{\lambda} (A + a)^{-2} \right).$$
(1.5)

We continue by rewriting the trace on the right in (1.5) using the Hilbert–Schmidt norm. We square the resulting inequality, use (1.3)-(1.4), and we obtain

$$\operatorname{Tr} P_{\lambda} \le (\lambda + a)^{2^{2}} \operatorname{Tr} \left(P_{\lambda} (A + a)^{-2^{2}} \right).$$
(1.6)

Continuing in this way, we obtain, for any $n \in \mathbb{N}$,

$$\operatorname{Tr} P_{\lambda} \le (\lambda + a)^{2^{n}} \operatorname{Tr} \left(P_{\lambda} (A + a)^{-2^{n}} \right).$$
(1.7)

This may also be written as

$$\operatorname{Tr}(P_{\lambda}(B+a)^{-2^{n}}) \leq \operatorname{Tr}(P_{\lambda}(A+a)^{-2^{n}}).$$
(1.8)

2. The restriction of B to the range of P_B has a compact resolvent since it is the fractional power of a positive trace class operator $P_B(B + A)^{-m}$. Consequently, the restriction BP_B has pure point spectrum so that $P_B = \sum_j P_{\lambda_j}$, with $BP_{\lambda_j} = \lambda_j P_{\lambda_j}$. If we take $2^n > m$, the assumption that $P_B(B + a)^{-m}$ is in the trace class implies that $\sum_j (\lambda_j + a)^{-2^n}$ is finite. Furthermore, since $P_B(A + a)^{-2^n}$ is in the trace class, if we truncate P_B to a finite N-dimensional subspace and call the truncated projector P_B^N , we have

$$\lim_{N \to \infty} \operatorname{Tr} \left(P_B^N (A+a)^{-2^n} \right) = \operatorname{Tr} \left(P_B (A+a)^{-2^n} \right).$$

As a consequence, we can sum the inequalities (1.8) over j to obtain

$$\operatorname{Tr}(P_B(B+a)^{-2^n}) \le \operatorname{Tr}(P_B(A+a)^{-2^n}).$$
(1.9)

This establishes the inequality in statement (1).

3. For the exponential bound, we use the truncation P_B^N of P_B , obtained by restricting P_B to an *N*-dimensional subspace, introduced above. For t > 0 and $b \in \mathbb{R}$ so that $b > -\inf \sigma(A)$, we obtain from the spectral theorem for *B* and inequality (1.7)

$$\operatorname{Tr} P_B^N e^{-t(B+b)} = \lim_{n \to \infty} \operatorname{Tr} \left[P_B^N \left(1 + \frac{t(B+b)}{2^n} \right)^{-2^n} \right]$$
$$\leq \lim_{n \to \infty} \operatorname{Tr} \left[P_B^N \left(1 + \frac{t(A+b)}{2^n} \right)^{-2^n} \right]$$
$$= \operatorname{Tr} P_B^N e^{-t(A+b)}. \tag{1.10}$$

It follows from the trace class property of $P_B e^{-tB}$ that

$$\lim_{N \to \infty} \operatorname{Tr} P_B^N e^{-t(B+b)} = \operatorname{Tr} P_B e^{-t(B+b)}.$$
 (1.11)

We obtain from this and (1.10)

$$\operatorname{Tr} P_B e^{-t(B+b)} \le \lim_{N \to \infty} \operatorname{Tr} P_B^N e^{-t(A+b)}.$$
(1.12)

If $P_B e^{-t(A+b)}$ is in the trace class, then the limit converges since

$$\lim_{N \to \infty} \operatorname{Tr} P_B^N e^{-t(A+b)} = \lim_{N \to \infty} \operatorname{Tr} P_B^N P_B e^{-t(A+b)} P_B = \operatorname{Tr} P_B e^{-t(A+b)}.$$
 (1.13)

Inequality (1.12) and (1.13) prove the second claim of the theorem.

2. An application to trace inequalities

Theorem 1.1 may be applied to a large class of functions of self-adjoint operators in order to obtain some inequalities relating traces of functions of self-adjoint operators.

Definition 2.1. A real-valued function g is in the class \mathcal{L} if there is a nonnegative σ -finite Borel measure ρ supported on $[0, \infty)$ so that for s > 0

$$g(s) = \int_0^\infty e^{-st} \, d\rho(t).$$
 (2.1)

Theorem 2.2. Let self-adjoint operators A, B and projector P_B be as in Theorem 1.1. Then for any $g \in \mathcal{L}$ such that $P_Bg(B)$ and $P_Bg(A)$ are in the trace class, one has

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$$\operatorname{Tr} P_B g(B) \le \operatorname{Tr} P_B g(A). \tag{2.2}$$

Proof. By the representation of g in (2.1) and the second inequality of Theorem 2.2, the assumptions imply that

$$\operatorname{Tr} P_B g(B) = \int_0^\infty \operatorname{Tr}(P_B e^{-tB}) d\rho(t)$$

$$\leq \int_0^\infty \operatorname{Tr}(P_B e^{-tA}) d\rho(t)$$

$$= \operatorname{Tr}(P_B g(A)). \qquad (2.3)$$

A particularly useful example of functions g are those related to powers of the resolvent of a self-adjoint operator.

Corollary 2.3. Let self-adjoint operators A, B and projector P_B be as in Theorem 1.1, and let $a > -\inf \sigma(A)$. For any $\beta > m$, where m is defined in Theorem 1.1, we have

$$\operatorname{Tr}(P_B(B+a)^{-\beta}) \le \operatorname{Tr}(P_B(A+a)^{-\beta}).$$
(2.4)

Proof. We use the Laplace transform formula valid for $\alpha > -1$ and $\Re z > 0$:

$$\frac{1}{z^{1+\alpha}} = \frac{1}{\Gamma(1+\alpha)} \int_0^\infty e^{-zt} t^\alpha \, dt.$$
(2.5)

This shows that the function $g(s) = s^{-\beta}$ is in the class \mathcal{L} for any $\beta > 0$. The result (2.4) follows from Theorem 2.2.

We conclude this section with the following generalization of Theorem 2.2. It presents a trace comparison theorem for the class \mathcal{L} of functions of self-adjoint operators.

Theorem 2.4. Let A and B be two lower semibounded self-adjoint operators satisfying the hypotheses of Theorem 1.1. Suppose that $g \in \mathcal{L}$ and $f \geq 0$ so that f(B)g(B) and f(B)g(A) are in the trace class. We then have

$$\operatorname{Tr}(f(B)g(B)) \leq \operatorname{Tr}(f(B)g(A)).$$
 (2.6)

Proof. Since f(B)g(B) is assumed to be trace class, the operator B must have pure point spectrum $\{\lambda_j\}$ on the support of the function fg. For any j, it follows from Theorem 1.1 that

$$\operatorname{Tr}(P_{\lambda_j}g(B)) \leq \operatorname{Tr}(P_{\lambda_j}g(A)),$$
(2.7)

where, as above, $BP_{\lambda_j} = \lambda_j P_{\lambda_j}$. Multiplying both sides of (2.7) by $f(\lambda_j) \ge 0$, and summing over j results in (2.6).

We remark that if g(B) is in the trace class, we may take f = 1 and obtain

$$\operatorname{Tr}(g(B)) \le \operatorname{Tr}(g(A)),$$
(2.8)

a result that also follows from the *Min-Max theorem* [10, Theorem XIII.1], since any function $g \in \mathcal{L}$ is decreasing.

3. A relation with operator monotone functions

The following class of functions was introduced by Löwner [9] in 1934 and is the object of his famous theorem that we now recall.

Definition 3.1. Let $J \subset \mathbb{R}$ be a finite interval or a half-line. A function $g: J \to \mathbb{R}$ is operator monotone increasing (respectively, decreasing) in J if for all pairs of self-adjoint operators A, B with spectrum in J the operator inequality $A \leq B$ implies the operator inequality $g(A) \leq g(B)$ (respectively $g(B) \leq g(A)$).

If g is operator monotone decreasing, then (2.6) holds for any $f \geq 0$ and for all pairs of operators $A \leq B$ such that f(B)g(B) and f(B)g(A) are in the trace class. Because of this, we study the relationship between operator monotone decreasing functions and the class \mathcal{L} of Definition 2.1. For simplicity, we assume that $J = \mathbb{R}^+$. We denote by \mathcal{I} (respectively, \mathcal{D}) the class of operator monotone increasing (respectively, decreasing) functions on \mathbb{R}^+ . The map $g \in \mathcal{D} \to \tilde{g} \in \mathcal{I}$ defined by $\tilde{g}(s) := g(1/s)$, for s > 0, is a bijective involution between \mathcal{D} and \mathcal{I} .

Löwner's theorem [9] (see also [1]-[3], [6], [7]) states that g is operator monotone increasing if and only if g has an analytic extension to the upper-half complex plane with a positive imaginary part (see [7, Theorem 5.4]). Such functions are known as Herglotz or Pick functions and have integral representations. For example, Hansen proved the following representation.

Lemma 3.2 ([7, Corollary 5.1]). Let \tilde{g} be a positive operator monotone increasing function on the half-line \mathbb{R}^+ . Then there exists a bounded, positive measure μ on \mathbb{R}^+ such that

$$\tilde{g}(s) = \int_{\mathbb{R}^+} \frac{s(1+\lambda)}{s+\lambda} \, d\mu(\lambda), \quad s > 0.$$
(3.1)

It follows easily from Kato's result (1.1) that any function on \mathbb{R}^+ with a representation as on the right of (3.1) is in the class \mathcal{I} . The difficult part of the proof of Löwner's Theorem is the converse.

Using the bijection $g \to \tilde{g}$ between \mathcal{D} and \mathcal{I} described above, it follows that if $f \in \mathcal{D}$, then f has a representation of the form

$$f(s) = \int_{\mathbb{R}^+} \frac{1+\lambda}{1+s\lambda} d\mu(\lambda), \quad s > 0,$$
(3.2)

for some bounded positive measure μ on \mathbb{R}^+ . Using the Laplace transform representation (2.3) with $\alpha = 0$, we may write f as

$$f(s) = \int_{\mathbb{R}^+} e^{-st} h(t) dt, \qquad (3.3)$$

where h is defined by

$$h(t) = \int_{\mathbb{R}^+} \left(1 + \frac{1}{\lambda} \right) e^{-\frac{t}{\lambda}} d\mu(\lambda).$$
(3.4)

The function $h \in L^1_{loc}(\mathbb{R}^+)$, so by Definition 2.1, the function $f \in \mathcal{L}$.

This shows that $\mathcal{D} \subset \mathcal{L}$. On the other hand, the functions on \mathbb{R}^+ such as $f(s) = e^{-as}$, with a > 0, or $f(s) = (s+a)^{-\rho}$, with $\rho > 1$ and a > 0, belong to the class \mathcal{L} but not to the class \mathcal{D} . As a consequence, we obtain the following theorem.

Theorem 3.3. The class of operator monotone decreasing functions \mathcal{D} is strictly contained in the class of functions \mathcal{L} .

4. An application to the proof of Wegner's estimate

We complete the proof of the Wegner estimate given in [4]. Since this method of proof seems to have been used in several subsequent papers, we wanted to present the complete argument. The Wegner estimate is an upper bound on the probability that a local random Hamiltonian has eigenvalues in a given energy interval. We considered a large cube Λ centered at the origin in \mathbb{R}^d with odd integer side length. We let $H_{\omega} := -\Delta + V_{\omega}$ be the random Schrödinger operator on $L^2(\mathbb{R}^d)$ with a standard Anderson-type random potential $V_{\omega} \geq 0$ (this condition can be removed). We denote by H_{Λ} the restriction of H_{ω} to Λ with Dirichlet boundary conditions. This operator has discrete spectrum. For any bounded interval $I = [I_{-}, I_{+}] \subset \mathbb{R}$, we let $E_{\Lambda}(I)$ be the spectral projection for H_{Λ} and interval I. The trace of this projection is finite and it is a random variable. The Wegner estimate proved in [4, Proposition 4.5] is

$$\mathbb{P}\{\operatorname{Tr} E_{\Lambda}(I) \ge 1\} \le C_W |I| |\Lambda|, \tag{4.1}$$

where $C_W > 0$ is a finite constant depending on I_+ .

The proof of the Wegner estimate in [4] depends on a comparison of the operator H_{Λ} to a direct sum of operators defined on unit cubes in Λ . Let $\Lambda = \text{Int } \{\bigcup_{j} \Lambda_1(j)\}$ be a decomposition of Λ into unit cubes centered at the lattice points $\tilde{\Lambda}$ of Λ . In the proof of Proposition 4.5 (see [4, Section 4]), we used the operator inequality

$$H_{\Lambda} \ge H_{N,\Lambda} \equiv -\bigoplus_{j} \Delta_{N,j},$$

$$(4.2)$$

where $-\Delta_{N,j}$ is the Neumann Laplacian on a unit cube centered at $j \in \Lambda \cap \mathbb{Z}^d$, if the boundary of the cube does not intersect the boundary of Λ , or the Laplacian with mixed Neumann–Dirichlet boundary conditions if the cube's boundary intersects the boundary of Λ . This inequality is valid only in the operator form sense. It cannot be used in conjunction with Jensen's inequality as done after equation (4.15) in [4] since the eigenfunctions ϕ_n of H_{Λ} are not in the operator domain of $H_{N,\Lambda}$.

We apply Theorem 1.1 in order to complete the proof of Wegner's estimate as stated in [4, Proposition 4.5]. We divide the set of indices $\tilde{\Lambda}$ of the unit cubes in Λ into two sets: The set $\partial \tilde{\Lambda}$ associated with unit cubes whose boundary intersects $\partial \Lambda$, and the set Int $\tilde{\Lambda}$ of interior points. We take $A = H_{N,\Lambda}$, as defined in (4.2), and $B = H_{\Lambda}$, the restriction of H to Λ with Dirichlet boundary conditions.

We verify conditions (1) and (2) of Theorem 1.1. As quadratic forms, we have $Q(B) := Q(H_{\Lambda}) = H_0^1(\Lambda)$, whereas $Q(A) := Q(H_{N,\Lambda}) = \{\bigoplus_{j \in \text{Int }\tilde{\Lambda}} H^1(\Lambda_1(j))\} \oplus \{\bigoplus_{j \in \partial \tilde{\Lambda}} H_M^1(\Lambda_1(j))\}$, where $H_M^1(\Lambda_1(j))$ consists of functions in $H^1(\Lambda_1(j))$ with Neumann boundary conditions along $\partial \Lambda \cap \partial \Lambda_1(j)$. It follows that $Q(H_{\Lambda}) \subset Q(H_{N,\Lambda})$. The second condition of Theorem 1.1 holds identically.

We have $\inf \sigma(A) = 0$ in this case. Then, with the notation of [4], the projection P_B is $E_{\Lambda}(I_{\eta})$. From part 2 of Theorem 1.1, we have

$$\operatorname{Tr} E_{\Lambda}(I_{\eta}) \leq e^{I_{\eta,+}} \operatorname{Tr} \left(E_{\Lambda}(I_{\eta}) e^{-H_{\Lambda}} \right)$$
$$\leq e^{I_{\eta,+}} \operatorname{Tr} \left(E_{\Lambda}(I_{\eta}) e^{-H_{N,\Lambda}} \right)$$
$$= e^{I_{\eta,+}} \left(\sum_{j \in \Lambda \cap \mathbb{Z}^{d}} \operatorname{Tr} \left(E_{\Lambda}(I_{\eta}) e^{\Delta_{N,j}} \chi_{j} \right) \right), \tag{4.3}$$

where χ_j is the characteristic function for the unit cube $\Lambda_1(j)$ centered at $j \in \mathbb{Z}^d$. In this way, we recover (4.16) of [4]. Following the remainder of the proof there, since the operators $-\Delta_{N,j}$ do not depend on the random variables, we expand the trace in the eigenfunctions of $-\Delta_{N,j}$ and apply the spectral averaging result [4, Corollary 4.2]. In this manner, one obtains (4.1). We refer the reader to [5] for a more general proof of the Wegner estimate.

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