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TRACE NORM ESTIMATES FOR PRODUCTS OF INTEGRAL OPERATORS AND DIFFUSION SEMIGROUPS

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We give trace norm estimates for products of integral operators and for diffusion semigroups. These are applied to differences of heat semigroups. A natural example of an integral operator with finite trace which is not trace class is given.

INTRODUCTION

We prove two trace class criteria. The first, Theorem 1, provides an estimate for the trace norm of the product of two integral operators. The second, Theorem 3, concerns differences of diffusion semigroups. Both results are inspired by the same circle of problems, namely the search for trace estimates for differences of heat semigroups, which in turn are a powerful tool in the investigation of spectral properties of the associated Hamiltonians. The according applications are indicated in Section 3. Let us now give a little more details concerning the following sections.

Section 1 is devoted to a proof of Theorem 1 which states that

$$\|AB\|_{tr} \leq \int \|A[\cdot,x]\|_2 \|B[x,\cdot]\|_2 dm(x),$$

if A, B are operators with kernels $A[\cdot,\cdot], B[\cdot,\cdot]$ and the L_2-norms in the integral are assumed to exist. As one immediately notices, this includes the well-known case that A, B are Hilbert-Schmidt, but it is much more general: The kernels A, B do not even have to define bounded operators in L_2. We then relate the above estimate to Corollary 2, which is the key to the results of the second section. There we treat differences of ultracontractive diffusion semigroups. The advantage of Theorem 3 in comparison with the results of [9] is the fact that we do not have to assume the validity of a Feynman–Kac formula or even the existence of a stochastic process. This enables the easy application to Neumann boundary problems given in Corollary 5. We end the third section by giving an example which clarifies some aspects of the trace norm estimates for semigroup differences: We show that an additional Dirichlet boundary condition on a set of finite capacity can lead to a semigroup difference which is not trace class, but is a Hilbert–Schmidt operator with finite trace. This shows that a conjecture in [9] is wrong. Moreover it appears to be the first "natural" example of an operator with positive continuous kernel and finite trace which, nevertheless, is not trace class.

1. INTEGRAL OPERATORS

We assume throughout that $(X, \mathfrak{A}, m)$ is a σ–finite measure space and we are concerned with trace class operators on $L_2 = L_2(X, \mathfrak{A}, m)$ which we denote by $\mathfrak{B}_1 = \mathfrak{B}_1(L_2)$. We use $\|\cdot\|_{tr}$ for the trace norm on $\mathfrak{B}_1$ and write $(\mathfrak{B}_2, (\cdot|\cdot)_{HS})$ for the Hilbert Schmidt operators, where

$$(A|B)_{HS} = \text{trace}(B^*A).$$

A measurable function $A[\cdot,\cdot] : X \times X \to \mathbb{C}$ such that

$$(Af|g) = \int\int A[x,y]f(y)\overline{g(x)}dm(x)dm(y),$$

or, equivalently,

$$Af(\cdot) = \int A[\cdot,y]f(y)dm(y)$$

is said to be a kernel for the operator A.

THEOREM 1 *Let $A, B : X \times X \to \mathbb{C}$ be measurable such that $A[\cdot,x], B[x,\cdot] \in L_2$ for a.e. $x \in X$ and*

$$\int \|A[\cdot,z]\|_2\|B[z,\cdot]\|_2 dm(z) < \infty. \tag{1}$$

Then there is a trace class operator $AB : L_2 \to L_2$ with kernel

$$AB[x,y] = \int A[x,z]B[z,y]dm(z)$$

such that

$$\|AB\|_{tr} \leq \int \|A[\cdot,z]\|_2\|B[z,\cdot]\|_2 dm(z) \tag{2}$$

PROOF. Set $h(z) := \|A[\cdot,z]\|_2, g(z) := \|B[z,\cdot]\|_2$. With the convention $g^{-1}(x) := 0$ where $g(x) = 0$, we write $M_{g^{-1}}$ for the corresponding multiplication operator. It follows that

$$AB = AM_{h^{-1}}M_{(hg)^{1/2}}M_{(hg)^{1/2}}M_{g^{-1}}B.$$

However $AM_{h^{-1}}M_{(hg)^{1/2}}$ and $M_{(hg)^{1/2}}M_{g^{-1}}B$ are Hilbert–Schmidt operators because of

$$\begin{aligned}&\int dx\int dz|A(x,z)h^{-1}(z)(hg)^{1/2}(z)|^2\\ &=\int dx\int dz|A(x,z)h^{-1/2}(z)g^{1/2}(z)|^2\\ &=\int g(z)h(z)dz<\infty,\end{aligned}$$

and a similar computation for the kernel of $M_{(hg)^{1/2}}M_{g^{-1}}B$. □

Remark: The estimate in (2) cannot be improved in general. There are examples where the right-hand side of (2) is equal to the trace norm. Take for instance

$$A(x,y)=a_1(x)a_2(y),B(x,y)=b_1(x)b_2(y),$$

where a_i, b_i are positive functions on X. Moreover assume $a_1, b_2 \in L_2(X)$, $\int a_2(z)b_1(z)dz =: (a_2|b_1) < \infty$. Then$AB$ is trace class and the estimate in (2) yields

$$\|AB\|_{tr}\le\|a_1\|_2\|b_2\|_2(a_2|b_1).$$

On the other hand

$$\|AB\|_{tr}\ge\|a_1\|_2\|b_2\|_2(a_2|b_1)=\int\|A[\cdot,z]\|_2\|B[z,\cdot]\|_2dm(z).$$

COROLLARY 2 *Let* $A \in \mathfrak{B}(L_1, L_2), B \in \mathfrak{B}(L_2, L_1)$ *and assume that there exists a* Φ *in* L_1 *such that* $|Bf| \le \Phi$ *for every* f *in the unit ball of* L_2. *Then*

$$\|AB\|_{tr}\le\|A\|\cdot\|\Phi\|_1.$$

PROOF: The Dunford–Pettis Theorem (as presented, e.g. in [6]) ensures the existence of a kernel for A s.t.

$$\operatorname{esssup}_{x\in X}\|A[\cdot,x]\|_2=\|A\|.$$

Moreover, B admits a kernel with the property

$$\int_X\|B[x,\cdot]\|_2dm(x)\le\|\Phi\|_1<\infty.$$

In fact, let $C := M_{\Phi^{-1}}B$. Then C maps L_2 to L_∞ with norm less than 1. The Dunford–Pettis Theorem (applied to the adjoint C' of C) implies the existence of a kernel such that $\operatorname{esssup}\|C[x,\cdot]\|_2 < \infty$. Therefore, $B[x,y] := \Phi(x)C[x,y]$ is a kernel for B with the asserted properties. Now an appeal to Theorem 1 gives the desired estimate. □

We want to remark that Corollary 2 first appeared in a slightly different form [9] (with a proof that relied on some abstract machinery). In the present form with a more elementary proof it was given in [10]. Corollary 2 will be the key to the results in the following section.

Apart from its applications in Section 3, it proved to be a very useful tool in the spectral theoretic investigations of [10].

The following observation how Theorem 1 can be deduced from Corollary 2 is due to a referee, whose suggestion is gratefully acknowledged:
Consider, in the notation from above,

$$\tilde{A}f(x) = \int h(z)^{-1}A[x,z]f(z)dm(z), \quad \tilde{B}f(z) = h(z)\int B[z,y]f(y)dm(y).$$

Then, under the assumptions of Theorem 1, Corollary 2 is applicable to $\tilde{A}, \tilde{B}$ and yields the result of Theorem 1 as $\tilde{A}\tilde{B} = AB$.

2. DIFFUSION SEMIGROUPS

We call a semigroup $U = (U(t); t \geq 0)$ a *diffusion semigroup* if the following conditions are satisfied

- $U(t) \in \mathfrak{B}(L_\infty)$ is positivity preserving for all $t \geq 0$, i.e. $U(t)f \geq 0$ for $f \geq 0, t \geq 0$.
- $U(t)$ induces a bounded operator on L_p for all $t \geq 0, p \in [1,\infty)$
- $U(t)$ is self adjoint on L_2 for $t \geq 0$.

If furthermore,

- $U(t)$ induces a bounded operator from L_1 to L_∞ for all $t > 0$

we speak of an *ultracontractive diffusion semigroup.* To simplify notation, we denote by $\|A\|_{p,q}$ the norm of an operator from L_p to L_q and we use

$$L_q := \{f; |f|^q \in L_1\}, \|f\|_q := \||f|^q\|_1$$

for $0 < q < 1$. There is a natural order for positivity preserving semigroups which comes from the order of functions, namely

$$V \leq U :\Longleftrightarrow \forall t \geq 0, f \geq 0 : V(t)f \leq U(t)f.$$

The main result of this section deals with differences of semigroups which obey this order relation.

THEOREM 3 *Assume that U, V are ultracontractive diffusion semigroups satisfying $V \leq U$ and set $D(t) := U(t) - V(t)$ for $t \geq 0$.
If $D(t)1 \in L_{1/2}$ for some $t > 0$ then*

$$\|U(2t) - V(2t)\|_{tr} \leq \|D(t)1\|_{1/2}\|D(t)\|_{1,\infty}^{1/2}(\|U(t)\|_{1,2} + \|V(t)\|_{1,2}).$$

We single out one step in the proof of Theorem 3 which can be thought of as a Cauchy–Schwarz inequality for positivity preserving operators. For integral operators it can easily be deduced from the usual Cauchy–Schwarz inequality. In the proof below we make essential use of the existence of a *lifting* for σ–finite measure spaces (see [6, 4] for background information).

LEMMA 4 *Assume that $A : L_\infty \to L_\infty$ is positivity preserving and induces a bounded operator from L_1 to L_∞. Then, for $f \in L_2$:*

$$|Af| \leq (A1)^{1/2} \cdot (A(|f|^2))^{1/2}.$$

PROOF. Observe first that by interpolation A is also bounded from L_2 to L_∞. Denote by $\mathfrak{L}_\infty$ the essentially bounded measurable functions (not equivalence classes!). Since m is σ–finite there exists a lifting Λ, by which we understand a linear multiplicative (hence order preserving) mapping

$$\Lambda : L_\infty \longrightarrow \mathfrak{L}_\infty,$$

such that Λf is a function in the equivalence class f. For fixed $x \in X$ set

$$q_x : L_2 \times L_2 \longrightarrow \mathbb{C}, q_x(f,g) := \Lambda(A(f\overline{g}))(x).$$

As Λ is linear and positive, q_x is a positive sesquilinear form. The Cauchy–Schwarz inequality implies

$$|\Lambda(A(f\overline{g}))(x)| \leq (\Lambda(A|f|^2)(x))^{1/2} \cdot (\Lambda(A|g|^2)(x))^{1/2}$$

for all $x \in X$. Since Λf is a representative of f, we may take $g \in L_2, 0 \leq g \leq 1$ in the last inequality and obtain

$$|A(fg)| \leq (A|f|^2)^{1/2} \cdot (A1)^{1/2},$$

since $Ag^2 \leq A1$. Approximating the constant function 1 from below by a sequence g_n such that $0 \leq g_n \leq 1, g_n \in L_2$ and taking the limit $n \to \infty$ gives the desired inequality. □

PROOF of Theorem 3. First note that, by the semigroup property of U and V,

$$D(2t) = U(t)D(t) + D(t)V(t).$$

By Lemma 4, for $\|f\|_2 \leq 1$,

$$\begin{aligned} |D(t)f(x)| &\leq (D(t)1(x))^{1/2} \cdot (D(t)|f|^2(x))^{1/2} \\ &\leq (D(t)1(x))^{1/2} \|D(t)\|_{1,\infty}^{1/2} =: \Phi(x). \end{aligned}$$

Hence we can apply Corollary 2 and obtain

$$\begin{aligned} \|U(t)D(t)\|_{tr} &\leq \|\Phi\|_1 \cdot \|U(t)\|_{1,2} \\ &= \|D(t)1\|_{1/2} \|D(t)\|_{1,\infty}^{1/2} \|U(t)\|_{1,2}. \end{aligned}$$

By the same arguments

$$\begin{aligned} \|D(t)V(t)\|_{tr} &= \|V(t)D(t)\|_{tr} \\ &\leq \|D(t)1\|_{1/2} \|D(t)\|_{1,\infty}^{1/2} \|V(t)\|_{1,2}, \end{aligned}$$

so that the asserted estimate follows. □

3. APPLICATIONS AND EXAMPLES

In this section we want to illustrate the above theorems by some applications. Although we are interested in more general Hamiltonians (see [2]) we restrict ourselves to the Laplacian on $\mathbb{R}^d$ in order to keep preliminary definitions and technicalities at a minimum. We denote the heat semigroup by $U(t) := e^{1/2\Delta t}$ and write $\Delta_\Sigma^D, \Delta_\Sigma^N$ for the Dirichlet, respectively Neumann Laplacian on an open set $\Sigma \subset \mathbb{R}^d$. The latter are selfadjoint operators on $L_2(\Sigma)$, and we extend the semigroups they generate in the obvious way to all of $L_2(\mathbb{R}^d) = L_2(\Sigma) \oplus L_2(\Sigma^c)$ by setting $U_\Sigma^D := e^{1/2\Delta_\Sigma^D t} \oplus 0$. With the analogous notation for the Neumann operator we note in passing that

$$U_\Sigma^D \leq U, U_\Sigma^D \leq U_\Sigma^N,$$

while $U_\Sigma^N \not\leq U$ apart from trivial cases. While U, U_Σ^D are always ultracontractive (see [1], Section 2.1, especially Example 2.1.8), this is not the case for U_Σ^N (the Neumann Laplacian need not even have compact resolvent). By $\mathbb{P}^x$ we denote the Wiener measure for particles starting in x and get:

COROLLARY 5 *Let* $\phi_{\Sigma,t} := \mathbb{P}^x\{X_s \in \Sigma^c$ *for some* $s \leq t\}$ *for any open* $\Sigma \subset \mathbb{R}^d$.

(1) $\|U(2t) - U_\Sigma^D(2t)\|_{tr} \leq c(t) \int \phi_{\Sigma,t}(x)^{1/2} dx.$

(2) *If* U_Σ^N *is ultracontractive, then*

$$\|U(2t) - U_\Sigma^N(2t)\|_{tr} \leq c(t) \int \phi_{\Sigma,t}(x)^{1/2} dx.$$

PROOF. By the Feynman–Kac formula ([3]),

$$U_\Sigma^D(t)1(x) = \mathbb{P}^x\{X_s \in \Sigma \text{ for all } s \leq t\} \leq \chi_\Sigma.$$

Consequently,

$$\begin{aligned}(U(t) - U_\Sigma^D(t))1(x) &= 1 - \mathbb{P}^x\{\ldots\} \\ &= \mathbb{P}^x\{X_s \in \Sigma^c \text{ for some } s \leq t\}.\end{aligned}$$

Theorem 3 implies

$$\|U(2t) - U_\Sigma^D(2t)\|_{tr} \leq c(t)\|\phi_{\Sigma,t}\|_{1/2},$$

proving (1). If , furthermore, U_Σ^N is ultracontractive, we can apply Theorem 3 to the difference $U_\Sigma^N - U_\Sigma^D$, since $U_\Sigma^N 1 = \chi_\Sigma$ and therefore

$$(U_\Sigma^N(t) - U_\Sigma^D(t))1 = \phi_{\Sigma,t}\chi_\Sigma.$$

This yields (2). □

We would like to mention that the Neumann heat semigroup is ultracontractive if Σ has the extension property (see [1], Theorem 2.4.4, p. 77). Another way to prove part (2) of the above Corollary would be to apply the analysis of [9] to the Dirichlet form generated by the Neumann Laplacian. In order to do so, one faces technical problems related with the

existence of an associated process.
In the situation of Corollary 5(1) it would be desirable to weaken the assumption on $\phi_{\Sigma,t}$ to the requirement $\phi_{\Sigma,t} \in L_1$, since the latter is fulfilled for all sets Σ satisfying $\text{cap}(\Sigma^c) < \infty$ (see the proof of the following lemma), which in turn is a quite natural condition. In [9] the corresponding statement was formulated as a conjecture. The following lemma and the subsequent example show, however, that $\text{cap}(\Sigma^c) < \infty$ does not imply $\|U(t)-U_\Sigma^D(t)\|_{tr} < \infty$. There is one more reason why we find this example quite interesting: From the results of [9] it is clear that the semigroup difference in question is a Hilbert–Schmidt operator with positive continuous kernel. Moreover, it is easy to see that its trace is finite. Thus, according to a remark of Simon, [7], Remark 2, p. 37 one would expect it to be trace class, which is not the case. To introduce our example we have to recall the definition of the Birman–Solomjak space

$$l_1(L_2) := \{f : \mathbb{R}^d \to \mathbb{R}; \sum_{\alpha\in\mathbb{Z}^d} (\int_{C_\alpha} |f(x)|^2 dx)^{1/2} < \infty\},$$

where C_α denotes the unit cube centered at α; see [7], p. 55.

LEMMA 6 *Assume that* $\Gamma := \Sigma^c$ *satisfies* $\text{cap}(\Gamma) < \infty$ *but* $\chi_\Gamma \notin l_1(L_2)$. *Then* $\phi_{\Sigma,t} \in L_1$ *but* $U(t) - U_\Sigma^D(t) \notin \mathfrak{B}_1$ *for any* $t > 0$.

PROOF. For the potential theoretic notions used in this proof we refer the reader to [5], Chapter 3. Recall that

$$\text{cap}(\Gamma) = \min\{\int |\nabla f|^2 + |f|^2 dx; f \in W_0^{1,2}, \tilde{f} \geq \chi_\Gamma\},$$

where $\tilde{f}$ denotes the quasi-continuous representative of f. The unique minimizing element e_Γ is called the 1-equilibrium potential of Γ and can be represented by

$$e_\Gamma(x) = \int G(x,y) d\nu_\Gamma(y),$$

where ν_Γ is a measure supported on Γ with total mass equal to the capacity of Γ, and $G(x,y)$ is the kernel of $(-\Delta+1)^{-1}$. Since $\int G(x,y)dx = (-\Delta+1)^{-1}1(y) = 1$,

$$\begin{aligned} \|e_\Gamma\|_1 &= \int\int G(x,y) d\nu_\Gamma(y) dx \\ &= \int (\int G(x,y)dx) d\nu_\Gamma \\ &= \text{cap}(\Gamma). \end{aligned}$$

(Put in potential theoretic terms, this calculation proves the equality of the 1-Dirichlet capacity cap and the 1-Newtonian capacity.) Denote $\tau(w) := \inf\{s > 0; X_s(w) \in \Gamma\}$, the first hitting time of Γ. Then

$$\phi_{\Sigma,t}(x) = \mathbb{E}^x\{\tau \leq t\} \leq e^t \mathbb{E}^x\{e^{-\tau}\} = e^t e_\Gamma(x),$$

where we used [5], Lemma 4.3.1 in the last step. This proves the first assertion. If $U(t) - U_\Sigma^D(t) \in \mathfrak{B}_1$ for some $t > 0$, it follows that $\chi_\Gamma(U(t) - U_\Sigma^D(t)) \in \mathfrak{B}_1$. Since

$\chi_\Gamma(U(t) - U_\Sigma^D(t)) = \chi_\Gamma U(t)$, we may apply [7], Proposition 4.7, to deduce $\chi_\Gamma \in l_1(L_2)$. □

EXAMPLE 7 *If $d \geq 5$ and $\Gamma := \bigcup_n B_n$, where B_n is a ball of radius r_n centered at $(n, 0 \ldots, 0)$ with $r_n \leq 1/2$ we have*

$$\mathrm{cap}(\Gamma) \leq c \sum_n r_n^{d-2}, \|\chi_\Gamma\|_{l_1(L_2)} = c' \sum_n r_n^{d/2}.$$

For $r_n = 1/2 \cdot n^{-2/d}$ it follows that $\mathrm{cap}(\Gamma) < \infty$ and $\chi_\Gamma \notin l_1(L_2)$. Consequently, $U(t) - U_\Sigma^D(t)$ is Hilbert–Schmidt with finite trace but not trace class.

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