AN OPTIMAL L^p-BOUND ON THE KREIN SPECTRAL SHIFT FUNCTION

By

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Dedicated to the memory of Tom Wolff, analyst extraordinaire and friend

Abstract. Let $\xi_{A,B}$ be the Krein spectral shift function for a pair of operators A, B, with $C = A - B$ trace class. We establish the bound

$$\int F(|\xi_{A,B}(\lambda)|)\,d\lambda \le \int F(|\xi_{|C|,0}(\lambda)|)\,d\lambda = \sum_{j=1}^{\infty} [F(j) - F(j-1)]\mu_j(C),$$

where F is any non-negative convex function on $[0, \infty)$ with $F(0) = 0$ and $\mu_j(C)$ are the singular values of C. The choice $F(t) = t^p$, $p \ge 1$, improves a recent bound of Combes, Hislop and Nakamura.

1 Introduction

Let A, B be bounded self-adjoint operators such that their difference $A - B$ is trace class. The Krein spectral shift function $\xi_{A,B}$ for the pair A, B is determined by

$$\operatorname{tr}(f(A) - f(B)) = \int f'(\lambda)\xi_{A,B}(\lambda)\,d\lambda$$

for all functions $f \in C_0^\infty(\mathbb{R})$ and $\xi(\lambda) = 0$ if $|\lambda|$ is large enough. The two bounds

$$\int |\xi_{A,B}(\lambda)|\,d\lambda \le \operatorname{tr}(|A - B|) \tag{1}$$

and

$$|\xi_{A,B}(\lambda)| \le n \qquad \text{if } A - B \text{ is rank } n \tag{2}$$

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are well known; see, for example, [8] or [9]. The Krein spectral shift function can also be defined for unbounded self-adjoint operators A, B and enjoys the same properties as long as their difference is trace class. The results of this paper extend to general unbounded operators A and B (as long as their difference is trace class) but for simplicity, we suppose that A and B are bounded. For applications of the spectral shift function in scattering theory, see, for example, the survey article [1].

The spectral shift function has also found applications in the theory of random Schrödinger operators. Kostrykin and Schrader [6, 7] constructed a spectral shift density for random Schrödinger operators with Anderson-type potentials. More recently, Combes, Hislop and Nakamura [2] realized that L^p-bounds on the Krein spectral shift function can serve as a basic tool for a proof of Hölder continuity of the integrated density of states for a large class of continuous random Schrödinger operators. In terms of the singular values of the difference $C = A - B$, their bound reads

$$\|\xi_{A,B}\|_p := \Big(\int |\xi_{A,B}(\lambda)|^p \, d\lambda \Big)^{1/p} \leq \sum_{j=1}^{\infty} \mu_j(C)^{1/p} \tag{3}$$

for $1 \leq p < \infty$. Note that (3) includes the endpoint cases (1) and (2) for $p = 1$ and and in the limit $p \to \infty$, respectively.

To see what type of bound is the correct one for an L^p-bound on the Krein spectral shift function, we consider a special case. Let C be a positive trace class operator with eigenvalues μ_j. Calculating

$$\operatorname{tr}[f(C) - f(0)] = \sum_{j=1}^{\infty} \int_0^{\mu_j} f'(\lambda) \, d\lambda,$$

we see that the spectral shift function for the pair $C, 0$ is simply given by

$$\xi_{C,0}(\lambda) = n \text{ if } \mu_{n+1} \leq \lambda < \mu_n \qquad \text{and} \qquad \xi_{C,0}(\lambda) = 0 \text{ if } \lambda < 0 \text{ or } \lambda \geq \mu_1. \tag{4}$$

For cases like this where A and B are finite rank, it is known that the spectral shift function is just the difference of the dimensions of the spectral subspaces — which leads immediately to another way of seeing why (4) is true. In particular, $\xi_{C,0}$ enjoys the following important properties:

- $\xi_{C,0}$ takes only values in $\mathbb{N}_0$ (or $\mathbb{Z}$ if C is not non-negative).
- For any non-negative function F on $[0, \infty)$ with $F(0) = 0$, we have

$$\int F(|\xi_{C,0}(\lambda)|) \, d\lambda = \sum_{j=1}^{\infty} F(j)(\mu_j - \mu_{j+1}). \tag{5}$$

- In addition, if F is monotone increasing, then

$$\int F(|\xi_{C,0}(\lambda)|)\,d\lambda = \sum_{j=1}^{\infty} [F(j) - F(j-1)]\mu_j. \tag{6}$$

The first two claims follow immediately from (4). Formally, the last claim follows from the second by summation by parts. However, since

$$\sum_{j=1}^{N} F(j)(\mu_j - \mu_{j+1}) = \sum_{j=1}^{N} (F(j) - F(j-1))\mu_j - F(N)\mu_{N+1},$$

this usually poses some growth restriction on $F(j)$ for passing to the limit $N \to \infty$. We prefer not to do this but to use positivity instead. Observe that

$$\begin{aligned}\sum_{j=1}^{\infty} F(j)(\mu_j - \mu_{j+1}) &= \sum_{j=1}^{\infty}\sum_{n=1}^{j} (F(n) - F(n-1))(\mu_j - \mu_{j+1}) \\ &= \sum_{1\le n\le j} (F(n) - F(n-1))(\mu_j - \mu_{j+1}).\end{aligned}$$

By the assumptions on F and μ_j, all terms in this double sum are non-negative. Hence we can use the Fubini–Tonelli theorem to interchange the summation and conclude

$$\begin{aligned}\sum_{j=1}^{\infty} F(j)(\mu_j - \mu_{j+1}) &= \sum_{n=1}^{\infty} (F(n) - F(n-1)) \sum_{j=n}^{\infty} (\mu_j - \mu_{j+1}) \\ &= \sum_{n=1}^{\infty} (F(n) - F(n-1))\mu_n,\end{aligned}$$

where we have used the fact that the last sum telescopes and $\mu_n \to 0$ as $n \to \infty$. In particular, the right-hand side of (5) and (6) is finite if and only if the other is and then they are equal. Below, we use this type of argument freely to do summation by parts without a priori bounds on the boundary terms. Alternatively, one could consider the case of finite rank operators $C = A - B$ first and then use some approximation arguments.

Our main result is that the above example (6) is an extreme case.

Theorem 1. *Let F be a non-negative convex function on $[0,\infty)$ vanishing at zero. Given a non-negative compact operator C with singular values $\mu_j(C)$, we have*

$$\begin{aligned}\int F(|\xi_{A,B}(\lambda)|)\,d\lambda &\le \int F(|\xi_{C,0}(\lambda)|)\,d\lambda \\ &= \sum_{j=1}^{\infty} [F(j) - F(j-1)]\mu_j(C)\end{aligned} \tag{7}$$

for all pairs of bounded operators A, B *with* $\sum_{j=n}^{\infty} \mu_j(|A-B|) \le \sum_{j=n}^{\infty} \mu_j(C)$ *for all* $n \in \mathbb{N}$. *In particular, this is the case if* $|A-B| \le C$.

Remark. Moreover, if F is strictly convex, the above inequality is strict if either the modulus of $\xi_{A,B}$ takes non-integer values on a set of positive Lebesgue measure or one does not have equality in Lemma 3 below. However, it seems to be difficult to find necessary and sufficient conditions on A and B alone for the case of equality in (7).

Specializing to $F(t) = t^p$ for some $p \ge 1$, we get

Corollary 2. *Let* $\xi_{A,B}$ *be the Krein spectral shift function for the pair* A, B. *In terms of the singular values* μ_j *of the difference* $A - B$, *we have the* L^p*-bound*

$$\|\xi_{A,B}\|_p \le \|\xi_{|A-B|,0}\|_p = \Big(\sum_{n=1}^{\infty} \big[n^p - (n-1)^p\big]\mu_n\Big)^{1/p}. \tag{8}$$

Remarks. (i) There are two different ways to see that (8) is, indeed, stronger than the bound (3) by Combes et al. First, the direct argument: rewrite

$$\Big(\sum_{n=1}^{\infty} \big[n^p - (n-1)^p\big]\mu_n\Big)^{1/p} = \Big(\sum_{n=1}^{\infty} n^p(\mu_n - \mu_{n+1})\Big)^{1/p}$$

and consider the right-hand side as the l^p-norm of the function $n \to n^p$ in the weighted l^p-space $l^p(\mu)$ with measure $\mu(n) := \mu_n - \mu_{n+1}$ for $n \in \mathbb{N}$. Write $n = 1+(n-1)$ and use Minkowski's inequality for the $l^p(\mu)$-norm to get

$$\begin{aligned}
\Big(\sum_{n=1}^{\infty} n^p\mu(n)\Big)^{1/p} &\le \Big(\sum_{n=1}^{\infty} \mu(n)\Big)^{1/p} + \Big(\sum_{n=2}^{\infty}(n-1)^p\mu(j)\Big)^{1/p} \\
&= \mu_1^{1/p} + \Big(\sum_{n=2}^{\infty}(n-1)^p\mu(n)\Big)^{1/p} \\
&\le \sum_{n=1}^{N} \mu_n^{1/p} + \Big(\sum_{n=N}^{\infty}(n-N)^p\mu(n)\Big)^{1/p},
\end{aligned}$$

where, for the last inequality, we have repeated the first step N times. Using monotone convergence for the limit $N \to \infty$, we conclude

$$\Big(\sum_{n=1}^{\infty} \big[n^p - (n-1)^p\big]\mu_n\Big)^{1/p} \le \sum_{n=1}^{\infty} \mu_n^{1/p}. \tag{9}$$

For the soft argument, note that, according to (6),

$$\Big(\sum_{n=1}^{\infty} \big[n^p - (n-1)^p\big]\mu_n\Big)^{1/p} = \|\xi_{C,0}\|_p,$$

where C is any non-negative compact operator with singular values μ_n. The bound (3) for $\xi_{C,0}$ immediately implies the inequality (9). Of course, the direct argument is, in some sense, a reformulation of the inductive proof of Combes et al.

(ii) Our result shows that if $\sum_{n=1}^{\infty} n^{p-1}\mu_n < \infty$, then $\xi_{A,B} \in L^p(\mathbb{R})$. Note that this *cannot* be improved insofar as only conditions on μ_n are used. It is also strictly better than the result by Combes et al. For example, if $\mu_n = n^{-p}\log(n+2)^{-\alpha}$, then Combes et al. require $\alpha > p$ to conclude $\xi_{A,B} \in L^p(\mathbb{R})$, while our result only needs $\alpha > 1$.

2 Two proofs

We give two proofs of our main result, Theorem 1, both depending on different aspects of the problem. First, some notation. For a complex-valued function f, let m_f be its distribution function, that is, $m_f(t) := |\{\lambda : |f(\lambda)| > t\}|$, with $|\mathcal{A}|$ the Lebesgue measure of a Borel set $\mathcal{A} \subset \mathbb{R}$. We write $m_{A,B}$ for the distribution function of $\xi_{A,B}$. The following lemma is the core of both proofs.

Lemma 3 (*Basic Lemma*). *With $C = A - B$, we have for all $n \in \mathbb{N}_0$*

$$\int_n^{\infty} m_{A,B}(t)\,dt \le \sum_{j=n+1}^{\infty} \mu_j(C) = \int_n^{\infty} m_{|C|,0}(t)\,dt.$$

Remark. Setting $(x-s)_+ := \sup\{0, x-s\}$, we have

$$\int_s^{\infty} m_f(t)\,dt = \int (|f(\lambda)| - s)_+\,d\lambda \tag{10}$$

for all $s \ge 0$. Hence Lemma 3 is equivalent to

$$\int (|\xi_{A,B}(\lambda)| - n)_+\,d\lambda \le \sum_{j=n+1}^{\infty} \mu_j(C) = \int (|\xi_{|C|,0}(\lambda)| - n)_+\,d\lambda.$$

Proof of Lemma 3. By the formula (4) for $\xi_{|C|,0}$,

$$\begin{aligned}\int (|\xi_{|C|,0}|(\lambda) - n)_+\,d\lambda &= \sum_{j=n+1}^{\infty} (j-n)(\mu_j - \mu_{j+1}) \\ &= \sum_{l=n+1}^{\infty}\sum_{j=l}^{\infty}(\mu_j - \mu_{j+1}) = \sum_{l=n+1}^{\infty} \mu_l,\end{aligned}$$

proving the second part of the assertion in the lemma.

For the inequality, let ψ_j, ϕ_j be two sets of orthonormal vectors such that $A - B = \sum_{j=1}^{\infty} \mu_j \langle \phi_j, \cdot \rangle \psi_j$. Note that $\phi_j = \pm\psi_j$ since A and B are self-adjoint.

Set $C_0 := 0$ and $C_n := \sum_{j=1}^{n} \mu_j \langle \phi_j, \cdot \rangle \psi_j$ for $n \in \mathbb{N}$. The spectral shift function is transitive. In particular,

$$\xi_{A,B} = \xi_{A,A+C_n} + \xi_{A+C_n,B}.$$

By (2), we know $|\xi_{A,A+C_n}| \le n$. Thus

$$(|\xi_{A,B}(\lambda)| - n)_+ \le |\xi_{A+C_n,B}(\lambda)|$$

and hence, by (10) and (1),

$$\int_n^\infty m_{A,B}(t)\,dt = \int (|\xi_{A,B}(\lambda)| - n)_+ \,d\lambda \le \operatorname{tr}|C - C_n| = \sum_{j=n+1}^{\infty} \mu_j.$$

□

In the following, we write m and ξ for $m_{A,B}$ and $\xi_{A,B}$, respectively.

First proof of Theorem 1. For $n \in \mathbb{N}_0$, put $a_n := F(n+1) - F(n)$, so that $F(n) = \sum_{0 \le l < n} a_l$. The a_n are monotone increasing by the convexity of F, that is, $a_n - a_{n-1} \ge 0$ for all $n \in \mathbb{N}$. Furthermore, set

$$x_n := \int_n^\infty m(t)\,dt$$

and observe that, by (10),

$$\int_{n<|\xi|\le n+1} (|\xi_{A,B}(\lambda)| - n)\,d\lambda = x_n - x_{n+1} - m(n+1). \tag{11}$$

Consider

$$\int F(|\xi(\lambda)|)\,d\lambda = \sum_{n=0}^{\infty} \int_{n<|\xi|\le n+1} F(|\xi(\lambda)|)\,d\lambda. \tag{12}$$

By the convexity of F, we have $F(s) \le F(n) + (s-n)\big(F(n+1) - F(n)\big)$ for $s \in [n, n+1]$.

Plugging this into (12), we obtain

$$\int F(|\xi(\lambda)|)\,d\lambda$$

$$\leq \sum_{n=0}^{\infty}\Big[F(n)\int_{n<|\xi|\leq n+1} d\lambda + a_n \int_{n<|\xi|\leq n+1} (|\xi(\lambda)|-n)\,d\lambda\Big]$$

$$= \sum_{n=0}^{\infty}\Big[\Big(\sum_{l=0}^{n-1} a_l\Big)\big(m(n)-m(n+1)\big) + a_n\big(x_n - x_{n+1} - m(n+1)\big)\Big] \text{ (by (11))}$$

$$(13)\quad = \sum_{l=0}^{\infty} a_l \sum_{n=l+1}^{\infty}\big(m(n)-m(n+1)\big) + \sum_{n=0}^{\infty} a_n\big(x_n - x_{n+1} - m(n+1)\big)$$

$$= \sum_{l=0}^{\infty} a_l m(l+1) + \sum_{n=0}^{\infty} a_n\big(x_n - x_{n+1} - m(n+1)\big)$$

$$= \sum_{n=0}^{\infty} a_n\big(x_n - x_{n+1}\big).$$

Note that if F is strictly convex, we have equality in this inequality if and only if ξ takes only integer values! Using that the terms in this sum are non-negative, we can again reorder the summations freely to conclude, setting $a_{-1} := 0$,

$$\int F(|\xi(\lambda)|)\,d\lambda \leq \sum_{n=0}^{\infty} a_n(x_n - x_{n+1}) = \sum_{0\leq l\leq n} (a_l - a_{l-1})(x_n - x_{n+1})$$

$$(14)\quad = \sum_{l=0}^{\infty}(a_l - a_{l-1})x_l \leq \sum_{l=0}^{\infty}(a_l - a_{l-1})\sum_{j=l+1}^{\infty}\mu_j$$

$$= \sum_{j=1}^{\infty}\big(F(j) - F(j-1)\big)\mu_j,$$

where in the last inequality we have used the positivity of the increments $a_l - a_{l-1}$ (aka convexity of F) and Lemma 3. This proves Theorem 1, including the case of equality since, if F is strictly convex and ξ takes non-integer values on a set of positive measure, the inequality in (13) is strict. We shall return to this question in our second proof. □

For the second proof we need some preparatory lemmas.

Lemma 4. *For any non-negative convex function F on $[0,\infty)$ which vanishes at zero, there exists a non-negative locally finite measure ν_F on $[0,\infty)$ such that*

$$F(t) = \int_0^{\infty} (t-u)_+ \nu_F(du) \quad \textit{for all } t \geq 0.$$

F is strictly convex if and only if ν_F is strictly positive, that is, $\nu_F([a,b]) > 0$ for all $0 \le a < b$.

Proof. Of course, this result is well-known. We give a short proof for completeness. Define $F(t)$ to be zero for negative t — it then becomes convex on all of $\mathbb{R}$. The assumptions on F show that the left derivative F' exists everywhere and is non-negative, monotone increasing, and continuous from the left. Hence it defines a measure ν_F by setting $\nu_F([a,b)) := F'(b) - F'(a)$. That this formula involves intervals which include a is a consequence of the left continuity of F' as we have defined it. Note that in this formula, $F'(0) = 0$ since it is the left derivative. The measure ν_F has a point mass at 0, which is precisely the right derivative of F at zero. This measure is strictly positive on $[0,\infty)$ if and only if F' is strictly increasing on $[0,\infty)$, that is, if and only if F is strictly convex. Moreover, by construction, $F'(s) = \nu_F([0,s))$ for all $s \ge 0$. Calculating

$$\begin{aligned}\int_0^\infty (t-u)_+ \nu_F(du) &= \int_{[0,t)} \int_u^t ds\, \nu_F(du) = \int_0^t \nu_F([0,s))\, ds \\ &= \int_0^t F'(s)\, ds = F(t)\end{aligned}$$

proves the assertion. □

Some more notation: recall that for a function f, $m_f(t) := |\{\lambda \mid |f(\lambda)| > t\}|$ and define

$$Q_f(s) := \int_s^\infty m_f(t)\, dt = \int (|f(\lambda)| - s)_+\, d\lambda. \tag{15}$$

Lemma 5. *Let F be any non-negative, convex function F on $[0,\infty)$ which vanishes at zero. Given two functions f and g, $Q_f \le Q_g$ implies*

$$\int F(|f(\lambda)|)\, d\lambda \le \int F(|g(\lambda)|)\, d\lambda.$$

Moreover, if F is strictly convex and $Q_f < Q_g$ on a set of positive Lebesgue measure, then the inequality above is strict.

Proof. From Lemma 4, we have

$$\int F(|f(\lambda)|)\, d\lambda = \int_0^\infty Q_f(u)\, \nu_F(du),$$

which concludes the proof. □

Remark. Necessary and sufficient conditions for the inequality in Lemma 5 to hold for all convex F have a long history, and Lemma 5 is implicit in the earliest papers on the subject by Hardy, Littlewood, Pólya [3] and Karamata [5]; see also Section 3.17 of [4].

Lemma 6. *Suppose that g takes only values in an unbounded, discrete set $\mathcal{S} \subset [0,\infty)$ with $0 \in \mathcal{S}$. Then the inequality $Q_f(s) \leq Q_g(s)$ for $s \in \mathcal{S}$ implies $Q_f(t) \leq Q_g(t)$ for all $t \in [0,\infty)$.*

Proof. Let $\mathcal{S} = \{0 = s_0 < s_1 < s_2 < \cdots\}$. Notice that Q_f is always convex and, furthermore, Q_g is linear on $[s_j, s_{j+1}]$. The claim follows from convexity since, by assumption, $Q_f(s) \leq Q_g(s)$ for $s \in \mathcal{S}$. □

Now we come to the

Second proof of Theorem 1. Given bounded operators A and B, let $D = |A - B|$ and C be any non-negative, compact, trace class operator with $\sum_{j=n}^{\infty} \mu_j(D) \leq \sum_{j=n}^{\infty} \mu_j(C)$ for all $n \in \mathbb{N}$. The basic Lemma 3 shows

$$Q_{\xi_{A,B}}(n) \leq Q_{\xi_{|D|,0}}(n) \leq Q_{\xi_{C,0}}(n) \quad \text{for all } n \in \mathbb{N}_0. \tag{16}$$

Lemma 6 then implies that (16) extends from $\mathbb{N}_0$ to all positive real n. Once one has that, Lemma 5 proves (7).

If $|\xi_{A,B}|$ takes non-integer values on a set of positive Lebesgue measure, then there exists $n \in \mathbb{N}_0$ such that $Q_{\xi_{A,B}}$ is strictly smaller than $Q_{\xi_{|D|,0}}$ on the interval $(n, n+1)$. This shows that if F is strictly convex, equality can hold only as long as $|\xi_{A,B}|$ is integer-valued. □

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References

[1] M. S. Birman and D. R. Yafaev, *The spectral shift function. The papers of M.G. Krein and their further development*, St. Petersburg Math. J. **4** (1993), 833–870.

[2] J.-M. Combes, P. Hislop and S. Nakamura, *The L^p-theory of the spectral shift function, the Wegner estimate, and the integrated density of states for some random operators*, preprint.

[3] G. H. Hardy, J. E. Littlewood and G. Pólya, *Some simple inequalities satisfied by convex functions*, Messenger of Math. **58** (1929), 145–152.

[4] G. H. Hardy, J. E. Littlewood and G. Pólya, *Inequalities*, Cambridge University Press, 1934.

[5] J. Karamata, *Sur une inégalité relative aux fonctions convexes*, Publ. Math. Univ. Belgrade **1** (1932), 145–148.

[6] V. Kostrykin and R. Schrader, *Scattering theory approach to random Schrödinger operators in one dimension*, Rev. Math. Phys. **11** (1999), 187–242.

[7] V. Kostrykin and R. Schrader, *The density of states and the spectral shift density of random Schrödinger operators*, Rev. Math. Phys., to appear.

[8] B. Simon, *Spectral analysis of rank one perturbations and applications*, CRM Proc. Lecture Notes **8** (J. Feldman, R. Froese and L. Rosen, eds.), Amer. Math. Soc., Providence, RI, 1995, pp. 109–149.

[9] D. R. Yafaev, *Mathematical Scattering Theory*, Amer. Math. Soc., Providence, RI, 1992.

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