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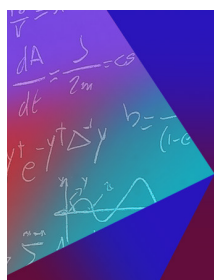
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A trace inequality of Ando, Hiai, and Okubo and a monotonicity property of the Golden–Thompson inequality

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ABSTRACT

The Golden–Thompson trace inequality, which states that $\text{Tr} e^{H+K} \leq \text{Tr} e^H e^K$, has proved to be very useful in quantum statistical mechanics. Golden used it to show that the classical free energy is less than the quantum one. Here, we make this G–T inequality more explicit by proving that for some operators, notably the operators of interest in quantum mechanics, $H = \Delta$ or $H = -\sqrt{-\Delta + m}$ and $K = \text{potential}$, $\text{Tr} e^{H+(1-u)K} e^{uK}$ is a monotone increasing function of the parameter u for $0 \leq u \leq 1$. Our proof utilizes an inequality of Ando, Hiai, and Okubo (AHO): $\text{Tr} X^s Y^t X^{1-s} Y^{1-t} \leq \text{Tr} XY$ for positive operators X, Y and for $\frac{1}{2} \leq s, t \leq 1$, and $s+t \leq \frac{3}{2}$. The obvious conjecture that this inequality should hold up to $s+t \leq 1$ was proved false by Plevnik [Indian J. Pure Appl. Math. 47, 491–500 (2016)]. We give a different proof of AHO and also give more counterexamples in the $\frac{3}{2}, 1$ range. More importantly, we show that the inequality conjectured in AHO does indeed hold in the full range if X, Y have a certain positivity property—one that does hold for quantum mechanical operators, thus enabling us to prove our G–T monotonicity theorem.

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I. INTRODUCTION

In 2000, Ando, Hiai, and Okubo² (AHO) considered several inequalities for traces of products of two positive semidefinite matrices X and Y , of which the two simplest were

$$|\text{Tr}[X^s Y^t X^{1-s} Y^{1-t}]| \leq \text{Tr}[XY] \quad (1.1)$$

and

$$\text{Tr}[X^{1/2} Y^{1/2} X^{1/2} Y^{1/2}] \leq |\text{Tr}[X^s Y^t X^{1-s} Y^{1-t}]| \quad (1.2)$$

with $1/2 \leq s \leq 1$ and $1/2 \leq t \leq 1$.

Note that the absolute value, or at least a real part, is necessary for either (1.1) or (1.2) to make sense; $\text{Tr}[X^s Y^t X^{1-s} Y^{1-t}]$ may be a complex number.

Ando, Hiai, and Okubo succeeded in proving both inequalities when X and Y were 2×2 matrices or, more generally, when both X and Y have at most two distinct eigenvalues (Ref. 2, Corollary 4.3). They also proved (1.1) when $s+t \leq 3/2$ but could only prove (1.2) when either $s = 1/2$ or $t = 1/2$. They raised the question as to whether the inequalities (1.1) and (1.2) hold over the entire range $1 \leq s+t \leq 2$. In addition to proving the positive results mentioned above (and some generalizations discussed below), they remarked that the behavior of the function $(s, t) \mapsto |\text{Tr}[X^s Y^t X^{1-s} Y^{1-t}]|$ on the whole interval $[1/2, 1] \times [1/2, 1]$ “is rather complicated for general $n \times n$ positive semidefinite matrices.”

The question they raised attracted the attention of other researchers. In particular, Bottazzi *et al.*⁵ gave another proof, for the case $s = t$, that (1.1) is valid for $s + t \leq 3/2$. Instead of the majorization techniques used in Ref. 2, they used the Lieb–Thirring inequality and the Hölder inequality for matrix trace norms. Using these tools, they showed that for $z = 1/4 + iy$ or $z = 3/4 + iy$, $y \in \mathbb{R}$,

$$|\mathrm{Tr}[X^z Y^z X^{1-z} Y^{1-z}]| \leq \mathrm{Tr}[XY] \quad (1.3)$$

and then used the maximum modulus principle to conclude that (1.1) is valid for $s = t$, $1/4 \leq t \leq 3/4$. Moreover, they proved that unless A and B commute, this inequality is strict, and thus, for any given X and Y , the inequality extends to a wider interval depending on X and Y . However, 16 years after the original work of Ando, Hiai, and Okubo, Plevnik⁹ finally found a counterexample to the conjectured inequality (1.1) in the missing range $3/2 \leq s + t \leq 2$, as well as a counterexample to (1.2).

We, unaware of these developments, attempted to show a monotonicity property for the Golden–Thompson inequality^{7,11} and were led to exactly the same inequality that Ando *et al.*² had discussed 22 years earlier. Our proof for the $1 \leq s + t \leq 3/2$ range is a little different, and we shall give that proof here. We also identify interesting conditions on X and Y under which (1.1) and (1.2) do hold for all $0 \leq s, t \leq 1$ and apply this to prove our conjecture on the Golden–Thompson inequality in these cases. We shall also give a systematic construction of counterexamples for the $3/2 \leq s + t \leq 2$ range that complement the example in Ref. 9 and show that not only is (1.2) false, but also it is even possible for $\mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}]$ to be negative when X and Y are real positive semidefinite matrices.

II. CONDITIONS FOR VALIDITY OF THE AHO INEQUALITIES

We recall the Lieb–Thirring inequality,⁸ which says that for all $r \geq 1$ and any positive semidefinite $n \times n$ matrices,

$$\mathrm{Tr}[(B^{-1/2} A B^{1/2})^r] \leq \mathrm{Tr}[A^r B^r]. \quad (2.1)$$

Later, Araki³ proved that the inequality reverses for $0 < r < 1$. It was shown by Friedland and So⁶ that for $r > 1$, the inequality is strict unless A and B commute.

In the following and in the whole of this paper, X and Y are positive semidefinite matrices. We will use (2.1) to estimate $\|X^{1/p} Y^{1/p}\|_p$ for various values of $p \geq 1$. Since

$$\|X^{1/p} Y^{1/p}\|_p^p = \mathrm{Tr}[(Y^{1/p} X^{2/p} Y^{1/p})^{p/2}],$$

we may apply (2.1) to get an upper bound on $\|X^{1/p} Y^{1/p}\|_p$ taking $r = p/2$, provided $p/2 \geq 1$ or, equivalently, $1/p \leq 1/2$. [Otherwise, by Araki's complement to (2.1), we would get a lower bound.] In summary,

$$\|X^{1/p} Y^{1/p}\|_p^p \leq \mathrm{Tr}[XY] \quad \text{for all } 0 < 1/p \leq 1/2. \quad (2.2)$$

As in Ref. 5, we shall use the generalized Hölder inequality for trace norms (see, e.g., Simon's book¹⁰). For any $3n \times n$ matrices A , B , and C and any $p, q, r \geq 1$ with $1/p + 1/q + 1/r = 1$,

$$|\mathrm{Tr}[ABC]| \leq \|ABC\|_1 \leq \|A\|_p \|B\|_q \|C\|_r. \quad (2.3)$$

(This generalizes in the obvious way to products of arbitrarily many matrices.)

The next theorem is a small generalization of the result in Ref. 2 in that we consider four positive semidefinite matrices instead of only two.

Theorem 2.1. *Let X , Y , Z , and W be positive semidefinite, and let $1/2 \leq s, t$, $t + s \leq 3/2$. Then,*

$$|\mathrm{Tr}[X^t Y^s Z^{1-t} W^{1-s}]| \leq (\mathrm{Tr}[XY])^{t+s-1} (\mathrm{Tr}[YZ])^{1-t} (\mathrm{Tr}[WX])^{1-s}. \quad (2.4)$$

In particular, taking $Z = X$ and $W = Y$, we obtain (1.1) under these conditions on s and t .

Proof. Since $s, t \geq 1/2$, $t \geq 1 - s$. Write $t = (1 - s) + (t + s - 1)$, and both summands are non-negative. By cyclicity of the trace,

$$\begin{aligned} \mathrm{Tr}[X^t Y^s Z^{1-t} W^{1-s}] &= \mathrm{Tr}[X^{t+s-1} Y^s Z^{1-t} W^{1-s} X^{1-s}] \\ &= \mathrm{Tr}[(X^{t+s-1} Y^{t+s-1})(Y^{1-t} Z^{1-t})(W^{1-s} X^{1-s})]. \end{aligned}$$

Define $r_1 := t + s - 1$, $r_2 := 1 - t$, and $r_3 := 1 - s$. Then, we have

$$\mathrm{Tr}[X^t Y^s Z^{1-t} W^{1-s}] = \mathrm{Tr}[(X^{r_1} Y^{r_1})(Y^{r_2} Z^{r_2})(W^{r_3} X^{r_3})].$$

By what was noted above, $r_1, r_2, r_3 \geq 0$, and of course, $r_1 + r_2 + r_3 = 1$. Thus, by Hölder's inequality,

$$|\mathrm{Tr}[X^t Y^s Z^{1-t} W^{1-s}]| \leq \|X^{r_1} Y^{r_1}\|_{1/r_1} \|Y^{r_2} Z^{r_2}\|_{1/r_2} \|W^{r_3} X^{r_3}\|_{1/r_3}. \quad (2.5)$$

We may now apply (2.2), provided r_1, r_2 , and r_3 are all no greater than $1/2$. Since $s, t \geq 1/2$, it is always the case that $r_2, r_3 \leq 1/2$, while $r_1 \leq 1/2$ if and only if $t + s \leq \frac{3}{2}$. Hence, under this condition, (2.4) is proved. $\square$

Remark 2.2. The assumption that the two powers of X sum to 1 is not a real restriction. Given two arbitrary positive powers a, b , we may rename X^{a+b} to be X and define $s := \max\{a, b\}/(a + b)$ and similarly for Y .

Remark 2.3. In Ref. 2, Theorem 2.1 was generalized to n X 's and n Y 's, and our method of Proof of Theorem 2.1 using the Lieb–Thirring inequality likewise generalizes. This theorem will not be needed in the rest of this paper, and we do not discuss this here.

Remark 2.4. The fact that this method of proof cannot yield the inequality for all s, t , even in cases such as those described below for which the inequality is true for all s, t , has nothing to do with what is given up in the application of the Lieb–Thirring inequality: Consider the case $s = t, Z = X$ and $W = Y$. Then, (2.5) becomes

$$|\mathrm{Tr}[X^t Y^t X^{1-t} Y^{1-t}]| \leq \|X^{2t-1} Y^{2t-1}\|_{1/(2t-1)} \|Y^{1-t} X^{1-t}\|_{1/(1-t)} \|Y^{1-t} X^{1-t}\|_{1/(1-t)}. \quad (2.6)$$

Hence, for $X, Y > 0$,

$$\lim_{t \uparrow 1} \|X^{2t-1} Y^{2t-1}\|_{1/(2t-1)} \|Y^{1-t} X^{1-t}\|_{1/(1-t)} \|Y^{1-t} X^{1-t}\|_{1/(1-t)} = \|XY\|_1,$$

and in general, $\|XY\|_1 > \mathrm{Tr}[XY]$.

We now present several results that provide conditions on X and Y under which (1.1) and (1.2) are valid for all $s, t \in [1/2, 1] \times [1/2, 1]$. We will use the following lemma:

Lemma 2.5. Suppose that X and s are such that in a basis in which Y is diagonal,

$$(X^s)_{ij} (X^{1-s})_{ji} \geq 0 \quad \text{for all } i, j. \quad (2.7)$$

Then, for all $t \in [1/2, 1]$,

$$\mathrm{Tr}[X^{1/2} Y^{1/2} X^{1/2} Y^{1/2}] \leq |\mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}]| \leq \mathrm{Tr}[XY]. \quad (2.8)$$

Remark 2.6. The matrix $M_{ij} := (X^s)_{ij} (X^{1-s})_{ji}$ is the Hadamard product of two positive matrices, namely, X^s and the transpose of X^{1-s} , and as such, it is positive semidefinite. However, the off-diagonal entries need not be positive or even real.

Proof. Assume first that $Y > 0$. Computing in any basis that diagonalizes Y , with the j th diagonal entry of Y denoted by y_j ,

$$f(t) := \mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}] = \sum_{ij} ((X^s)_{ij} (X^{1-s})_{ji}) y_j^t y_i^{1-t},$$

where now it is convenient to let t range over $[0, 1]$. Under hypothesis (2.7), $f(t)$ is symmetric and convex in t . Hence, its maximum occurs at $t = 0$ and $t = 1$, and its minimum occurs at $t = 1/2$. Since $Y > 0$, $\lim_{t \uparrow 1} \mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}] = \mathrm{Tr}[X^s Y X^{1-s}] = \mathrm{Tr}[XY]$. This proves that $\mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}]$ is real and satisfies

$$\mathrm{Tr}[X^s Y^{1/2} X^{1-s} Y^{1/2}] \leq |\mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}]| \leq \mathrm{Tr}[XY].$$

Since $(Y^{1/2})_{ij} (Y^{1/2})_{ji} = |Y_{ij}^{1/2}|^2$, we may now apply what was proved above with the roles of X and Y interchanged to conclude that

$$\mathrm{Tr}[X^{1/2} Y^{1/2} X^{1/2} Y^{1/2}] \leq \mathrm{Tr}[X^s Y^{1/2} X^{1-s} Y^{1/2}].$$

Finally, we obtain the same result assuming only $Y \geq 0$ using the obvious limiting argument. $\square$

Our first application of Lemma 2.5 is to pairs of operators of a sort that arise frequently in mathematical physics. For $X > 0$, define $H = -\log(X)$ so that $X = e^{-H}$. Suppose that in a basis in which Y is diagonal, all off-diagonal entries of H are non-positive, i.e.,

$$H_{ij} \leq 0 \quad \text{for all } i \neq j. \quad (2.9)$$

For example, this is the case if H is the graph Laplacian on an unoriented graph (with the graph theorist's sign convention that the graph Laplacian is non-negative); see Example 3.3.

It is well-known that under these conditions, as a consequence of the Beurling–Deny Theorem (Ref. 4, Theorem 5), the semigroup e^{-sH} is positivity preserving, and so, in particular, $(e^{-sH})_{ij} \geq 0$ for all s and all i, j . For the reader's convenience, we recall the relevant part of their proof adapted to our setting: Take $\lambda > 0$ sufficiently small that $I + \lambda H$ is invertible. Then, for any vector f , $(I + \lambda H)^{-1}f$ is the unique minimizer of

$$F(u) := \lambda \langle u, Hu \rangle + \|u - f\|^2.$$

The uniqueness follows from the strict convexity of F for sufficiently small $\lambda > 0$. Under condition (2.9), when $f = |f|$, $F(|u|) \leq F(u)$. Hence, $(I + \lambda H)^{-1}f$ maps the positive cone into itself, and all entries of this matrix are non-negative. The same is evidently true of $(I + \lambda H)^{-n}f$ for all n . Taking $\lambda = s/n$ and $n \rightarrow \infty$, the same is true of e^{-sH} for all $s \geq 0$.

Theorem 2.7. Suppose that $H = -\log X$ satisfies (2.9) in a basis in which Y is diagonal. Then, (1.1) and (1.2) are valid for all $s, t \in [1/2, 1]$.

Proof. By the Beurling–Deny theorem as explained above, for all $s > 0$,

$$(X^s)_{ij} = (e^{-sH})_{ij} \geq 0.$$

It follows that (2.7) is satisfied for all s , and now the conclusion follows from Lemma 2.5. $\square$

One may also use Lemma 2.5 to show that both (1.1) and (1.2) are valid for 2×2 matrices, as was already shown in Ref. 2: Write $X = \begin{bmatrix} a & z \\ \bar{z} & b \end{bmatrix}$. Then, by the usual integral representation formula for X^s , $0 < s < 1$,

$$(X^s)_{1,2} = -z \left(\frac{\sin(\pi\alpha)}{\pi} \int_0^\infty \lambda^s \frac{1}{(a+\lambda)(b+\lambda) - |z|^2} d\lambda \right),$$

showing that for all $0 < \alpha < 1$, $(Y^\alpha)_{1,2}$ is a positive multiple of $-z$, and hence, (2.7) is always true.

Our next theorem provides another class of examples of positive matrices X and Y for which (1.1) is true for all $1/2 \leq s, t \leq 1$. A related theorem, for a version of (1.1) with the operator norm in place of the trace, has recently been proved in Ref. 1 by quite different means.

Theorem 2.8. Let H and K be arbitrary self-adjoint $n \times n$ matrices. Then, there exists an $\alpha_0 > 0$ depending on H and K so that for all $\alpha < \alpha_0$, with $X := e^{\alpha H}$ and $Y := e^{\alpha K}$, (1.1) is valid all $1/2 \leq s, t \leq 1$.

Proof. If H and K commute, then it is obvious that (1.1) is valid all $1/2 \leq s, t \leq 1$, no matter what $\alpha > 0$ may be. Hence, we may assume without loss of generality that $[H, K] \neq 0$. In addition, without loss of generality, we may suppose that H and K are both contractions and $0 \leq \alpha \leq 1$. Then, by the spectral theorem,

$$\left\| e^{\alpha H} - \left(I + \alpha H + \frac{\alpha^2}{2} H^2 \right) \right\| \leq e^\alpha \frac{\alpha^3}{6},$$

and likewise for K . Thus,

$$\left\| e^{\alpha H} e^{\alpha K} - \left(I + \alpha H + \frac{\alpha^2}{2} H^2 \right) \left(I + \alpha K + \frac{\alpha^2}{2} K^2 \right) \right\| \leq e^{2\alpha} \frac{\alpha^3}{2}. \quad (2.10)$$

Note that

$$\begin{aligned} & \left(I + \alpha H + \frac{\alpha^2}{2} H^2 \right) \left(I + \alpha K + \frac{\alpha^2}{2} K^2 \right) \\ &= I + \alpha(H + K) + \frac{\alpha^2}{2}(H + K)^2 + \frac{\alpha^2}{2}[H, K] + R, \end{aligned} \quad (2.11)$$

where $\|R\| \leq 3\alpha^3$.

Now, writing $X = e^{\alpha H}$ and $Y = e^{\alpha K}$,

$$\text{Tr}[X^{1-s} Y^{1-t} X^s Y^t] = \text{Tr}[XYZ], \quad \text{where} \quad Z(s, t) := Y^{-t} X^s Y^t X^{-s}.$$

Using (2.10) and (2.11), we obtain

$$\|Z(s, t) - (I + \alpha^2 st[H, K])\| \leq C\alpha^3 \quad (2.12)$$

for some constant C that can be easily estimated. Note that for all s, t , $Z(0, t) = Z(s, 0) = I$. For this reason, there cannot be any terms proportional to s^2 or t^2 in the second order expansion.

Altogether we have

$$\begin{aligned}\mathrm{Tr}[X^{1-t}Y^{1-s}X^tY^s] &= \mathrm{Tr}\left[\left(I + (K+H) + \frac{1}{2}(K+H)^2 + \frac{1}{2}[H, K]\right)(I + st[H, K])\right] + R_2 \\ &= \mathrm{Tr}[XY] \\ &\quad + st\mathrm{Tr}\left[\left(I + \alpha(K+H) + \frac{\alpha^2}{2}(K+H)^2 + \frac{\alpha^2}{2}[H, K]\right)[H, K]\right] + R_3,\end{aligned}$$

where $\|R_2\|, \|R_3\| \leq C\alpha^3$ for some constant C . Evidently, $\mathrm{Tr}[[H, K]] = \mathrm{Tr}[[H[H, K]]] = \mathrm{Tr}[K[H, K]] = \mathrm{Tr}[[H^2[H, K]]] = \mathrm{Tr}[K^2[H, K]] = 0$. A simple computation shows that

$$\mathrm{Tr}[(HK + KH)(HK - KH)] = 0.$$

Therefore,

$$\mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] - \mathrm{Tr}[XY] + st\alpha^2\mathrm{Tr}[H, K]^2 + \mathrm{Tr}[R_4],$$

where $\|R_4\| \leq C\alpha^3$, and hence, $\mathrm{Tr}[R_4] \leq nC\alpha^3$. Evidently, since by hypothesis $[H, K] \neq 0$, $\mathrm{Tr}[H, K]^2 < 0$. Thus, for all α sufficiently small, $\mathrm{Tr}[X^{1-t}Y^{1-s}X^tY^s] - \mathrm{Tr}[XY] < 0$ for all $(s, t) \in [1/2, 1] \times [1/2, 1]$. $\square$

Of course, replacing t by $1-t$ and s by $1-s$, the same proof shows, with the same α_0 that when $\alpha \leq \alpha_0$,

$$\mathrm{Tr}[X^{1-t}Y^{1-s}X^tY^s] = \mathrm{Tr}[XY] + st\alpha^2\mathrm{Tr}[H, K]^2 \pm C\alpha^3.$$

Replacing s by is and t by it yields

$$\mathrm{Tr}[X^{1-is}Y^{1-it}X^{is}Y^{it}] = \mathrm{Tr}[XY] - (st)^2\mathrm{Tr}[H, K]^2 + \mathcal{O}(\delta^6),$$

and hence, $[X, Y] \neq 0$, and α sufficiently small,

$$\mathrm{Tr}[X^{1-it}Y^{1-is}X^{it}Y^{is}] > \mathrm{Tr}[XY].$$

Thus, the three lines argument in Ref. 5 cannot hold for s, t sufficiently close to 1 or 0.

III. THE MONOTONICITY OF THE GOLDEN-THOMPSON INEQUALITY

Let H and K be self-adjoint $n \times n$ matrices. For $0 \leq u \leq 1$, define

$$f_{H,K}(u) = \mathrm{Tr}[e^{H+(1-u)K}e^{uK}]. \quad (3.1)$$

Then, $f(0) = \mathrm{Tr}[e^{H+K}]$ and $f(1) = \mathrm{Tr}[e^He^K]$, and by the Golden-Thompson inequality,

$$\mathrm{Tr}[e^{H+K}] \leq \mathrm{Tr}[e^He^K], \quad (3.2)$$

$f_{H,K}(0) \leq f_{H,K}(1)$. In this section, we ask the following: When is $f_{H,K}(u)$ monotone increasing in u ? We shall prove that this is the case for an interesting class of pairs (H, K) of self-adjoint matrices, and we shall show that it is not true in general.

Remark 3.1. Observe that if one replaces H by $H + aI$ and K by $K + bI$,

$$f_{H+aI, K+bI}(u) = e^{a+b} f_{H,K}(u), \quad (3.3)$$

and hence, whether or not $f_{H+aI, K+bI}(u)$ is monotone increasing is independent of a and b .

Theorem 3.2. Suppose that K is diagonal and that all off-diagonal entries of H are non-negative. Then, $f_{H,K}(u)$ is monotone increasing.

Proof. By Remark 3.1, we may assume that $K \geq 0$. It will be convenient to define $H_u = H + (1-u)K$. Then,

$$\begin{aligned}f'(u) &= \mathrm{Tr}[e^{H_u}Ke^{uK}] - \int_0^1 \mathrm{Tr}[e^{(1-t)H_u}Ke^{tH_u}e^{uK}]dt \\ &= \sum_{m=0}^{\infty} \frac{u^m}{m!} \left(\mathrm{Tr}[e^{H_u}K^{m+1}] - \int_0^1 \mathrm{Tr}[e^{(1-t)H_u}Ke^{tH_u}K^m]dt \right).\end{aligned} \quad (3.4)$$

Now define $X = e^{H_u}$, and for each m , $Y = K^{m+1}$ and $s = (m+1)^{-1}$. With these definitions,

$$\mathrm{Tr}[e^{H_u} K^{m+1}] - \int_0^1 \mathrm{Tr}[e^{(1-t)H_u} K e^{tH_u} K^m] dt = \mathrm{Tr}[BA] - \int_0^1 \mathrm{Tr}[B^{1-t} A^s B^t A^{1-s}] dt.$$

Since Y is diagonal, for each u , $-\log H_u$ has non-positive off-diagonal entries. By Theorem 2.7,

$$\mathrm{Tr}[BA] - \int_0^1 \mathrm{Tr}[B^{1-t} A^s B^t A^{1-s}] dt \geq 0.$$

Then, by (3.4), $f'(u) \geq 0$. □

Example 3.3. Let $\mathcal{G}$ be a graph with a finite set of vertices $\mathcal{V}$. Let the edge set be $\mathcal{E}$; this is a subset of $\mathcal{V} \times \mathcal{V}$. Suppose that $\mathcal{G}$ is a simple graph, meaning that $(x, x) \notin \mathcal{E}$ for all $x \in \mathcal{V}$ and that $(x, y) \in \mathcal{E}$ if and only if $(y, x) \in \mathcal{E}$. Then, the graph Laplacian, $\Delta_{\mathcal{G}}$, is defined by

$$\Delta_{\mathcal{G}} f(x) = \sum_{\{y : (x, y) \in \mathcal{E}\}} (f(x) - f(y)).$$

In the natural basis, all off diagonal elements of the matrix representing $\Delta_{\mathcal{G}}$ are non-positive. Define $H_0 = \Delta_{\mathcal{G}}$ to obtain a non-negative “free Hamiltonian” as in the usual mathematical physics convention. Let V be a self-adjoint multiplication operator on $L^2(\mathcal{V}, \mu)$, where μ is the uniform probability measure on $\mathcal{V}$. In the natural basis, V is diagonal.

Then, by Theorem 3.2,

$$f(u) := \mathrm{Tr}[e^{-(H_0 + (1-u)V)} e^{-uV}]$$

is strictly monotone increasing in u .

Example 3.4. Although we have given proofs in the context of matrices, it is easy to see that the proofs extend to cover interesting infinite dimensional cases. Let $X = e^{\beta\Delta}$, where Δ is the Laplacian on $\mathbb{R}^d$ and $\beta > 0$. Let V be a real valued function on $\mathbb{R}^d$, and let V also denote multiplication by V acting on $L^2(\mathbb{R}^d)$, which is, in general, unbounded. Let $Y = e^{-\beta V}$. Then, since X^t has a positive kernel and Y acts by multiplication on $L^2(\mathbb{R}^d)$, the Proof of Theorem 3.2 is easily adapted to show that

$$f(u) := \mathrm{Tr}[e^{-\beta(\Delta + (1-u)V)} e^{-\beta u V}]$$

is monotone increasing in u . The same applies with $-\Delta$ replaced by $(-\Delta)^{1/2}$, another case that arises in physical applications.

IV. COUNTEREXAMPLES

This section presents the construction of counterexamples, showing that inequalities (1.1) and (1.2) cannot hold in general, even in the 3×3 case and showing the monotonicity property established in Theorem 3.2 under specified conditions cannot hold in general. While counterexamples for (1.1) and (1.2) were found by Plevnik,⁹ our goal is to provide a systematic approach to their construction. Plevnik provided two completely separate and purely numerical counterexamples to (1.1) and (1.2). We provide a method for constructing a family of counterexamples that goes further in significant ways. For example, while Plevnik showed in Ref. 9 (Example 2.5) that (1.2) can be violated, his example does not show that it is possible for $\mathrm{Tr}[X^s Y^t X^{1-s} Y^{1-t}]$ to be negative. We show that this is the case. Moreover, our construction shows that the failure of inequalities (1.1) and (1.2) as well as the failure, in general, of the monotonicity of the Golden–Thompson inequality described in Theorem 3.2 are all closely connected. Essentially, one example undoes all three would-be conjectures.

We have seen in Lemma 2.5 that if all of the entries of $M_{ij} := (X^s)_{ij} (X^{1-s})_{ji}$ are non-negative, then (1.1) and (1.2) both hold. In constructing our counterexamples, we shall take X to be real, and hence, the entries of M will be real for each s .

Lemma 4.1. Let $y := (y_1, \dots, y_n)$ be any vector in $\mathbb{R}^n$. Let X be any positive semidefinite $n \times n$ matrix, and let $0 \leq t \leq 1$. Let $M(s)$ denote the matrix $M_{ij}(s) := (X^s)_{ij} (X^{1-s})_{ji}$. Then, for all $0 < s < 1$,

$$\sum_{i,j=1}^n M_{ij}(s) (y_i - y_j)^2 \geq 0. \quad (4.1)$$

Proof. We may assume that the entries of y are positive since the left-hand side of (4.1) does not change when we add to y any multiple of the vector each of whose entries is 1.

By Lemma 2.5, we know that for X and any matrix $Y \geq 0$ (we replace Y by Y^2 in Lemma 2.5 for convenience),

$$\mathrm{Tr}[X^{1-s}YX^sY] \leq \mathrm{Tr}[XY^2] = \mathrm{Tr}[Y^2X].$$

Letting Y be the diagonal matrix whose j th diagonal entry is y_j , this becomes

$$\mathrm{Tr}[X^{1-s}YX^sY] = \sum_{i,j=1}^n y_i M_{ij}(s) y_j = \sum_{i,j=1}^n y_j M_{ij}(s) y_i \leq \sum_{i,j=1}^n y_i^2 M_{ij}(s) = \sum_{i,j=1}^n M_{ij}(s) y_j^2.$$

□

We now claim that if $X \geq 0$ is a real 3×3 matrix, for any $0 < s < 1$, $M(s)$ has at most one entry above the diagonal that is negative. [By Remark 2.6, all diagonal entries are non-negative, and $M(s)$ is symmetric, so the same is true below the diagonal.] To see this, take the vector y to be of the form $(0, 1, 1)$, $(1, 0, 1)$ or $(1, 1, 0)$. Then, for these choices, (4.1) becomes

$$2(M_{1,2}(s) + M_{1,3}(s)) \geq 0, \quad 2(M_{1,2}(s) + M_{2,3}(s)) \geq 0, \quad \text{and} \quad 2(M_{1,3}(s) + M_{2,3}(s)) \geq 0. \quad (4.2)$$

Thus, each pair of entries above the diagonal must have a non-negative sum, and hence, no two can be negative.

One might hope that one could construct counterexamples to (1.1) and (1.2) by constructing matrices $X > 0$ for which $M_{ij}(t) < 0$ for all $t \in (0, 1/2) \cup (1/2, 1)$. This is easy to do, but this alone does not yield counterexamples.

For example, define $X^{1/2} = \begin{bmatrix} 2 & \sqrt{2} & 0 \\ \sqrt{2} & 2 & \sqrt{2} \\ 0 & \sqrt{2} & 2 \end{bmatrix}$. This matrix is easily diagonalized; the eigenvalues are 4, 2, and 0. Since $X_{1,3}^{1/2} = 0$, one might expect that $X_{1,3}^s$ changes sign at $s = 1/2$, and only there so that $M_{1,3}(s) \leq 0$ for all $0 < s < 1$. Indeed, doing the computations, one finds

$$M_{1,3}(s) = -\frac{4^{-s}}{2}(4^s - 2)^2 \leq 0, \quad \text{while} \quad M_{1,1}(s) = M_{3,3}(s) = \frac{4^{-s}}{2}(4^s + 2)^2. \quad (4.3)$$

Now take $Y := \begin{bmatrix} a & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & b \end{bmatrix}$ with $a, b > 0$ and distinct. Then,

$$\mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] = M_{1,1}(s)a + M_{3,3}(s)b + M_{1,3}(s)(a^{1-t}b^t + a^tb^{1-t}). \quad (4.4)$$

For fixed $s \notin \{0, 1/2, 1\}$, this is strictly concave in t and symmetric about $t = 1/2$, so the maximum occurs only at $t = 1/2$ and the minimum only at $t \in \{0, 1\}$. However, since $\lim_{t \downarrow 0} Y^t = P := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \neq I$, we do not have $\lim_{t \downarrow 0} \mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] = \mathrm{Tr}[XY]$, which would provide a counterexample to (1.1) but instead $\lim_{t \downarrow 0} \mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] = \mathrm{Tr}[X^{1-s}YX^sP]$. As we have just seen, this is less than $\mathrm{Tr}[X^{1-s}Y^{1/2}X^sY^{1/2}]$, and by Lemma 2.5, this, in turn, is less than $\mathrm{Tr}[XY]$. In fact, defining $h(t) := 4^{t-1/2} + 4^{1/2-t}$, we can rewrite (4.3) as

$$M_{1,3}(s) = 2 - h(s) \quad \text{and} \quad M_{1,1}(s) = M_{3,3}(s) = 2 + h(s). \quad (4.5)$$

Then, from (4.4),

$$\mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] = 2(a + b + a^tb^{1-t} + a^{1-t}b^t) + h(s)(a + b - a^tb^{1-t} - a^{1-t}b^t). \quad (4.6)$$

By the arithmetic-geometric mean inequality, $a + b - a^tb^{1-t} - a^{1-t}b^t \geq 0$ for all $0 \leq t \leq 1$. Since $h(s)$ is evidently convex and symmetric about $s = 1/2$, for each fixed $t \in (0, 1)$, $\mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t]$ is a strictly convex function of s , symmetric about $s = 1/2$. Therefore, this function is minimized only for $s = 1/2$ and maximized only for $s \in \{0, 1\}$, and hence, for any t ,

$$\mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] \geq \mathrm{Tr}[X^{1/2}Y^{1-t}X^{1/2}Y^t],$$

and the right side is independent of t since $X_{1,3}^{1/2} = 0$. Hence, (1.2) is satisfied for all choices of $a, b > 0$. Likewise, by what was proved above, for all s, t , with $Q := \lim_{t \downarrow 0} X^s$, which is an orthogonal projection,

$$\mathrm{Tr}[X^{1-s}Y^{1-t}X^sY^t] \leq \mathrm{Tr}[X^{1-s}Y^{1/2}X^sY^{1/2}] \leq \mathrm{Tr}[QY^{1/2}X^1Y^{1/2}] \leq \mathrm{Tr}[XY],$$

and hence, (1.1) is satisfied for all choices of $a, b > 0$.

This shows that the construction of counterexamples is more subtle than simply producing negative entries in $M(s)$. It appears that the key to the construction of counterexamples for 3×3 matrices is to choose X so that one of the inequalities in (4.1) is nearly saturated, with one of the summands negative for most values of s . Furthermore, it is natural to choose X and Y to be perturbations of positive semidefinite

matrices X_0 and Y_0 such that $\text{Tr}[X_0^{1-s}Y_0^{1-t}X_0^sY_0^t] = 0$ for all $0 \leq s, t \leq 1$. Of course, this is satisfied if X_0 and Y_0 are orthogonal projections with mutually orthogonal ranges.

Our construction relies on the *Householder reflections* determined by two distinct unit vectors $u, v \in \mathbb{R}^n$. This is given by $H_{u,v} := I - 2\frac{\|u-v\|^{-1}|u-v\rangle\langle u-v|}$. Evidently, $H_{u,v}$ is self-adjoint, orthogonal, and $H_{u,v}u = v$ and $H_{u,v}v = u$. For simplicity, choose

$$u := (0, 0, 1) \quad \text{and} \quad v := 2^{-1/2}(1, 1, 0). \quad (4.7)$$

Then,

$$U := H_{u,v} = \frac{1}{2} \begin{bmatrix} 1 & -1 & \sqrt{2} \\ -1 & 1 & \sqrt{2} \\ \sqrt{2} & \sqrt{2} & 0 \end{bmatrix}.$$

Now choose

$$Y_0 := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad X_0 = UY_0U = \frac{1}{2} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

Then, X_0 and Y_0 are orthogonal projections such that $X_0Y_0 = 0$.

Now, we make a simple perturbation. For $a, b > 0$ small, to be chosen later, define

$$A := \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad Y := \begin{bmatrix} c & 0 & 0 \\ 0 & d & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

and also for $0 < t < 1$, define

$$\alpha := \frac{1}{4}(a^t + b^t) \quad \text{and} \quad \beta := \frac{\sqrt{2}}{4}(a^t - b^t).$$

Then,

$$UAU = X_0 + \begin{bmatrix} \alpha & -\alpha & \beta \\ -\alpha & \alpha & -\beta \\ \beta & -\beta & 2\alpha \end{bmatrix}.$$

The off-diagonal entries of UYU will not change sign as t varies, but we can make this happen by applying a further orthogonal transformation; define $R := \begin{bmatrix} \cos x & 0 & -\sin x \\ 0 & 1 & 0 \\ \sin x & 0 & \cos x \end{bmatrix}$, and finally put

$$X := RUAUR^T,$$

where R^T is the transpose of R , with x , a , and b to be chosen later. We compute

$$X_{1,3}^t = (\cos^2 x - \sin^2 x)\beta(t) + \sin x \cos x \left(\frac{1}{2} - \alpha(t) \right)$$

and

$$X_{2,3}^t = -\cos(x)\beta(t) + \sin x \left(\frac{1}{2} - \alpha(t) \right).$$

We seek a small perturbation of X_0 , and hence, we will take a , b , and $|x|$ all to be small positive numbers. It is easy to see that the sign change we seek occurs in $X_{1,3}^t$ if we take $a \ll b \ll 1$ and $0 < x \ll 1$, and occurs in $X_{2,3}^t$ if we take $b \ll a \ll 1$ and $0 < x \ll 1$.

Example 4.2. To get a counterexample to (1.1), take $a = 10^{-10}$, $b = 10^{-19}$, $x = 10^{-5}$, $c = 10^{-10}$ and $d = 0$. Then, one finds

$$\text{Tr}[XY] < 1.5001 \times 10^{-10}, \quad \text{while} \quad \text{Tr}[X^{0.79}Y^{0.79}X^{0.21}Y^{0.21}] > 1.61022 \times 10^{-10}.$$

Example 4.3. To get a counterexample to (1.2), take $a = 10^{-19}$, $b = 10^{-10}$, $x = 10^{-5}$, $c = 10^{-10}$, and $d = 0$. Then, one finds that

$$\mathrm{Tr}[X^{0.98} Y^{0.98} X^{0.02} Y^{0.02}] < -2.386\,74,$$

which being negative, is certainly less than $\mathrm{Tr}[X^{1/2} Y^{1/2} X^{1/2} Y^{1/2}] > 0$, and by continuity, somewhere the trace must be zero.

Note that the only difference between the two examples is that we have swapped the values assigned to a and b ; all other parameters are left the same. Numerical plots show that in both cases, the maximum value of $|M_{1,3}(t) + M_{2,3}(t)|$ is less than 10^{-3} times the maximum of $|M_{1,3}(t)| + |M_{2,3}(t)|$ so that the last inequality in (4.1) is nearly saturated; there is near cancellation in the sum $X_{1,3}^t + X_{2,3}^t$. Note that in our counterexample to (1.1), the sum of the exponents $s + t$ is 1.58, not so much larger than the minimum value, $3/2$, at which such a counterexample cannot exist. It would be of interest to see if one can build on this construction, possibly extending it into higher dimensions, to show that the condition $s + t \leq 3/2$ in Theorem 2.1 is sharp.

We close by showing that the monotonicity property for the Golden–Thompson inequality described in Theorem 3.2 does not hold for arbitrary self-adjoint matrices H and K .

Recall that $f_{H,K}(u)$ has been defined by (3.1),

$$f_{H,K}(u) = \mathrm{Tr}[e^{H+(1-u)K} e^{uK}], \quad (4.8)$$

$$\left. \frac{d}{du} f_{H,K}(u) \right|_{u=1} = \mathrm{Tr}[e^H K e^K] - \int_0^1 \mathrm{Tr}[e^{tH} K e^{(1-t)H} e^K] dt.$$

With X and Y as above, we define $K = \log(X)$ and $H = \log Y$. Since H is diagonal, the integral $\int_0^1 e^{tH} K e^{(1-t)H} dt$ can be explicitly evaluated as a Hadamard product. One finds

$$\left. \frac{d}{du} f_{H,K}(u) \right|_{u=1} < -3 \times 10^{-6}.$$

This shows that the monotonicity proved in Theorem 3.2 is not true for general self-adjoint H and K .

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Eric A. Carlen: Conceptualization (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal). **Elliott H. Lieb:** Conceptualization (equal); Investigation (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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