The Order Relation and Trace Inequalities for Hermitian Operators

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Abstract

In this paper, we give the order relation and trace inequalities of Hermitian operators by comparison with their counterparts of real numbers.

Keywords: Hermitian operators, order relation, trace inequalities

1 Introduction

Hermitian operators play an important role in mathematics and some scientific areas. In quantum information theory, they are frequently encountered [1]. Because Hermitian operators have real eigenvalues, they can be seen as the counterpart of real numbers. For example, there exists comparison relation between any two real numbers so that we can know which number is larger than the other. Likewise, we can define the order relation for Hermitian operators. In this paper, we will present the order relation and some trace inequalities of Hermitian operators by comparison with their counterparts of real numbers.
2 Preliminaries

In this paper, we assume that all operators are in one Hilbert space. The symbol “†” stands for Hermitian adjoint operation and the symbol “∗” stands for complex conjugate operation.

Suppose \( A \) is an operator on Hilbert space \( H \). We have the following definitions of three types of special operators [1].

**Definition 2.1** \( A \) is a **Hermitian operator** if \( A^\dagger = A \).

**Definition 2.2** \( A \) is a **positive operator** if for any vector \( |\psi\rangle \) in \( H \),
\[
\langle \psi | A | \psi \rangle \geq 0.
\]

**Definition 2.3** \( A \) is a **projection operator** if it has the form \( A = \sum_{i=1}^{k} |i\rangle \langle i| \) where \( \{|i\rangle\} \) is an orthonormal set in \( H \).

**Lemma 2.1** Suppose \( A \) is an operator on Hilbert space \( H \), then for any vector \( |\psi\rangle \) in \( H \), \( \langle \psi | A | \psi \rangle = 0 \) if and only if \( A = 0 \).

**Proof**
The converse is obvious.

For the forward statement, suppose \( \langle \psi | A | \psi \rangle = 0 \) for any vector \( |\psi\rangle \) in \( H \).

Because any operator \( A \) on one Hilbert space can be written as \( A = B + iC \) where \( B = \frac{1}{2}(A + A^\dagger) \) and \( C = \frac{1}{2i}(A - A^\dagger) \) are both Hermitian operators. Thus
\[
\langle \psi | A | \psi \rangle = 0 \Leftrightarrow \langle \psi | (B + iC) | \psi \rangle = 0 \Leftrightarrow \langle \psi | B | \psi \rangle + i \langle \psi | C | \psi \rangle = 0.
\]

For a Hermitian operator \( H \) and an arbitrary vector \( |\psi\rangle \), the complex conjugate of the complex number \( \langle \psi | H | \psi \rangle \) is \( \langle \psi | H | \psi \rangle^* = \langle \psi | H | \psi \rangle^\dagger = \langle \psi | H | \psi \rangle \), thus \( \langle \psi | H | \psi \rangle \) is real. So both \( \langle \psi | B | \psi \rangle \) and \( \langle \psi | C | \psi \rangle \) are all real numbers.

Therefore
\[
\langle \psi | B | \psi \rangle + i \langle \psi | C | \psi \rangle = 0 \Leftrightarrow \langle \psi | B | \psi \rangle = \langle \psi | C | \psi \rangle = 0.
\]
Because \(|\psi\rangle\) is arbitrary, we can choose one eigenvector \(|v\rangle\) corresponding to any eigenvalue \(\lambda\) of \(B\). Hence \(\langle v|B|v\rangle = \lambda \|v\|^2 = 0 \Rightarrow \lambda = 0\). Thus all eigenvalues of \(B\) are zeros. By the spectral decomposition of \(B\), we immediately get \(B = 0\). Similarly, \(C = 0\). Therefore \(A = B + iC = 0\).

Note that we can conclude all eigenvalues of \(A\) are zeros directly from the condition “\(\langle \psi |A|\psi \rangle = 0\) for all \(|\psi\rangle\) in \(H\)” by the similar way above (replace \(|\psi\rangle\) by one eigenvector of any eigenvalue of \(A\)) without writing it as \(A = B + iC\).

But can we get \(A = 0\) from this fact? The answer is negative. The reason arises from the fact that all eigenvalues of one operator are zeros is not sufficient to ensure this operator is definitely a zero operator. For example, the operator \(|1\rangle\langle 0|\) on a qubit, which has matrix representation
\[
\begin{pmatrix}
0 & 0 \\
1 & 0
\end{pmatrix}
\]
with respect to the basis \(|0\rangle,|1\rangle\}, has only zero eigenvalues. But \(|1\rangle\langle 0| \neq 0\). Hence, although we can conclude that all eigenvalues of \(A\) are zeros, we cannot get \(A = 0\) unless \(A\) has a spectral decomposition like the Hermitian operators \(B\) and \(C\) in the proof of this lemma. This is why we write \(A\) as \(A = B + iC\) with two Hermitian operators \(B\) and \(C\).

**Theorem 2.1** Suppose \(A\) is an operator on Hilbert space \(H\), then for any vector \(|\psi\rangle\) in \(H\), \(\langle \psi |A|\psi \rangle\) is a real number if and only if \(A\) is a Hermitian operator.

**Proof**

The converse has been shown in the proof of Lemma 2.1.

For the forward statement, if \(\langle \psi |A|\psi \rangle\) is a real number for any vector \(|\psi\rangle\) in \(H\), equivalently we have
\[
\langle \psi |A|\psi \rangle^* = \langle \psi |A|\psi \rangle \iff \langle \psi |A|\psi \rangle^\dagger = \langle \psi |A|\psi \rangle \iff \langle \psi |A^\dagger|\psi \rangle = \langle \psi |A|\psi \rangle \iff \\
\langle \psi |(A^\dagger - A)|\psi \rangle = 0 .
\]
By Lemma 2.1, we get
\[ A^\dagger - A = 0 \iff A^\dagger = A \iff A \text{ is a Hermitian operator.} \]

**Corollary 2.1** A positive operator is necessarily a Hermitian operator.

**Proof**
Suppose \( A \) is a positive operator satisfying, by Definition 2.2, \( \langle \psi \vert A \psi \rangle \) is real and non-negative for any vector \( \vert \psi \rangle \) in one Hilbert space. So by Theorem 2.1, \( A \) is a Hermitian operator.

By Definition 2.3 and Corollary 2.1, it is easy to verify that a projection operator is necessarily a positive operator and hence a Hermitian operator. We can find from Lemma 2.1, Definition 2.2 and Theorem 2.1 that the equivalent conditions for the zero operator, positive operators and Hermitian operators all focus on the same number \( \langle \psi \vert A \psi \rangle \), where \( \vert \psi \rangle \) is arbitrary, and differ from each other only on taking a special value of \( \langle \psi \vert A \psi \rangle \), which is 0, a non-negative real number and a real number, respectively.

### 3 Order relation and trace inequalities for Hermitian operators

In this section, we restrict all operators to be Hermitian operators.

#### 3.1 Order relation for Hermitian operators

Hermitian operators have real eigenvalues. Hence, they can be seen as the counterpart of real numbers. We have the concept of the “larger” and “smaller” comparison between any two real numbers as well as inequalities for real numbers. Naturally, we expect that this kind of notion of comparison relation can be extended from real numbers to Hermitian operators. Consequently, there are inequalities for Hermitian operators. In fact, we can establish this notion as follows.

**Definition 3.1.1** Suppose both \( A \) and \( B \) are Hermitian operators. We write \( A \geq 0 \) if \( A \) is a positive operator. In addition, we write \( A \geq B \) if \( A - B \geq 0 \). Equivalently, we may write the inverse relation \( B \leq A \) if \( A \geq B \).

One can readily verify the operation properties of Hermitian operators and positive operators as follows:
If both $A$ and $B$ are Hermitian operators and $c$ is a real number, then

1. both $A + B$ and $A - B$ are Hermitian operators;
2. $cA$ is a Hermitian operator.

If both $A$ and $B$ are positive operators, and $c$ is a non-negative real number, i.e. if $A \geq 0$, $B \geq 0$, and $c \geq 0$, then

(i) $A + B \geq 0$;
(ii) $cA \geq 0$.

**Example 3.1.1** A projection operator $P$, by Definition 2.3, satisfies $0 \leq P \leq I$ where $I$ is the identity operator.

**Example 3.1.2** The three Pauli operators

$$
\sigma_x = |0\rangle\langle 1| + |1\rangle\langle 0|,
$$

$$
\sigma_y = i|1\rangle\langle 0| - i|0\rangle\langle 1|,
$$

and

$$
\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|
$$

which are three Hermitian operators satisfy

$$
-I \leq \sigma_x \leq I, \quad -I \leq \sigma_y \leq I, \quad -I \leq \sigma_z \leq I.
$$

To see this point and for simplicity, we denote any of these three Pauli operators as $\sigma$. Since $\sigma$ has eigenvalues $\pm 1$, it has spectral decomposition

$$
\sigma = |+1\rangle\langle +1| - |-1\rangle\langle -1|
$$

where $|+1\rangle$ and $|-1\rangle$ are orthonormal eigenvectors corresponding to eigenvalues $+1$ and $-1$, respectively. On the other hand,

$$
I = |+1\rangle\langle +1| + |-1\rangle\langle -1|.
$$

Thus

$$
\sigma - (-I) = 2|+1\rangle\langle +1| \geq 0 \quad \text{and} \quad I - \sigma = 2|-1\rangle\langle -1| \geq 0.
$$

Therefore

$$
-I \leq \sigma \leq I.
$$

**Property 3.1.1 (reflexive property)** The order relation $\leq$ for Hermitian operators is reflexive, i.e. for any Hermitian operator $A$, $A \leq A$.

**Proof**

Since for any Hermitian operator $A$, $A - A = 0$ where the zero operator $0$ is a positive operator. Thus by Definition 3.1, $A \leq A$.

**Property 3.1.2 (transitive property)** The order relation $\leq$ for Hermitian operators is transitive, i.e. If $A_1 \leq A_2$ and $A_2 \leq A_3$, then $A_1 \leq A_3$. 

□
Proof

If \( A_1 \leq A_2 \) and \( A_2 \leq A_3 \), then \( A_3 - A_1 = (A_3 - A_2) + (A_2 - A_1) \geq 0 \).

Hence \( A_1 \leq A_3 \).

\[ \square \]

Property 3.1.3 (antisymmetric property) \( A \leq B \) and \( B \leq A \) imply that \( A = B \).

Proof

By definition,

\[ A \leq B \iff \langle \psi | (B - A) | \psi \rangle \geq 0 \text{ for any } | \psi \rangle \]

and

\[ B \leq A \iff \langle \psi | (B - A) | \psi \rangle \leq 0 \text{ for any } | \psi \rangle . \]

Thus

\[ \langle \psi | (B - A) | \psi \rangle = 0 \text{ for any } | \psi \rangle . \]

By Lemma 2.1, we get \( A = B \).

These three properties of order relation for Hermitian operators are completely similar to those of order relation for real numbers. However, unlike real numbers, not every pair of Hermitian operators is comparable. For example, there exists no order relation between Hermitian operators \( A = |0\rangle\langle 0| \) and \( B = |1\rangle\langle 1| \), because neither \( A - B = |0\rangle\langle 0| - |1\rangle\langle 1| \) nor \( B - A = |1\rangle\langle 1| - |0\rangle\langle 0| \) is a positive operator (note that \( \langle 0 | (A - B) | 0 \rangle > 0 \), \( \langle 1 | (A - B) | 1 \rangle < 0 \), \( \langle 0 | (B - A) | 0 \rangle < 0 \), and \( \langle 1 | (B - A) | 1 \rangle > 0 \)) so that neither \( A \geq B \) nor \( B \geq A \) is true. In this sense, we can draw the conclusion:

Theorem 3.1.1 The order relation \( \leq \) for Hermitian operators is a partial order rather than a total order.

3.2 The trace inequalities for Hermitian operators

Although Hermitian operators can be seen as the counterpart of real numbers, when it comes to the multiplication operation, they are quite distinct from each other. The product of any two real numbers is definitely a real number. However, the product of two Hermitian operators may not be a Hermitian operator again.
One usual counterexample for this case is that the product of any two different Pauli operators in \( \{ \sigma_x, \sigma_y, \sigma_z \} \) is not a Hermitian operator but actually a skew-Hermitian operator (an operator \( A \) is a \textit{skew-Hermitian operator} if \( A^\dagger = -A \)). For example, \( \sigma_x \sigma_y = i \sigma_z \), where \( i \sigma_z \) has non-real but purely imaginary eigenvalues \( \pm i \), which implies that the product \( \sigma_x \sigma_y \) is not a Hermitian operator. Nevertheless, what is the result if we consider taking the \textit{trace} function (the \textit{trace} of an operator is the sum of all its eigenvalues) of the product of two Hermitian operators instead of the product itself? For instance, we check the last counterexample. We have \( tr(\sigma_x \sigma_y) = tr(i \sigma_z) = 0 \) (note that every Pauli operator in \( \{ \sigma_x, \sigma_y, \sigma_z \} \) has eigenvalues \( \pm 1 \)). The result \( 0 \) is a real number. Is that a fact rather than chance? Next we will show that it is actually a reality. Moreover, by using the spectral decomposition, we will prove and establish some trace inequalities for Hermitian operators and mainly for the product of two Hermitian operators which are similar to corresponding inequalities for real numbers.

**Theorem 3.2.1** If both \( A \) and \( B \) are Hermitian operators, then \( tr(AB) \) is a real number.

**Proof**

Since \( B \) is a Hermitian operator, it has the spectral decomposition \( B = \sum_i \lambda_i |i\rangle \langle i| \) with real eigenvalues \( \lambda_i \) and corresponding orthonormal eigenvectors \( |i\rangle \).

Thus \( tr(AB) = tr(A \sum_i \lambda_i |i\rangle \langle i|) = \sum_i \lambda_i tr(A |i\rangle \langle i|) = \sum_i \lambda_i \langle i|A|i\rangle \).

Since \( A \) is a Hermitian operator, \( \langle i|A|i\rangle \) is a real number for any \( i \) by Theorem 2.1. Therefore \( tr(AB) \) is a real number.

This result indicates that the product of two Hermitian operators may not be a Hermitian operator, while the trace of their product, however, is always a real number. But this fact does not hold for the product of three or more Hermitian
operators. For instance, \( \text{tr}(\sigma_x \sigma_y \sigma_z) = 2i \).

Based on this theorem, we will prove the following inequalities.

**Theorem 3.2.2 (The trace inequalities for Hermitian operators)**

If all operators in the following statements are Hermitian operators, we have inequalities below:

1. If \( A \leq B \), then \( \text{tr}(A) \leq \text{tr}(B) \);

2. If \( A \geq 0 \) and \( B \geq 0 \), then \( \text{tr}(AB) \geq 0 \);

3. If \( B \leq C \) and \( A \geq 0 \), then \( \text{tr}(BA) \leq \text{tr}(CA) \) and \( \text{tr}(AB) \leq \text{tr}(AC) \);

4. If \( 0 \leq A \leq A' \) and \( 0 \leq B \leq B' \), then \( 0 \leq \text{tr}(AB) \leq \text{tr}(A'B') \).

**Proof**

1. \( A \leq B \iff B - A \geq 0 \Rightarrow \text{tr}(B - A) \geq 0 \iff \text{tr}(B) - \text{tr}(A) \geq 0 \iff \text{tr}(A) \leq \text{tr}(B) \).

2. Since \( B \) is a positive operator, it has the spectral decomposition \( B = \sum_i \lambda_i \ket{i} \bra{i} \) with non-negative eigenvalues \( \lambda_i \) and corresponding orthonormal eigenvectors \( \ket{i} \).

Thus \( \text{tr}(AB) = \text{tr}(A \sum_i \lambda_i \ket{i} \bra{i}) = \sum_i \lambda_i \text{tr}(A \ket{i} \bra{i}) = \sum_i \lambda_i \bra{i} A \ket{i} \).

Since \( A \) is a positive operator, \( \bra{i} A \ket{i} \) is non-negative for any \( i \). Therefore \( \text{tr}(AB) \geq 0 \).

3. \( B \leq C \iff C - B \geq 0 \). By (2), \( \text{tr}((C - B)A) \geq 0 \iff \text{tr}(CA) - \text{tr}(BA) \geq 0 \iff \text{tr}(BA) \leq \text{tr}(CA) \). Similarly (or by \( \text{tr}(AB) = \text{tr}(BA) \) and \( \text{tr}(AC) = \text{tr}(CA) \)), we can obtain \( \text{tr}(AB) \leq \text{tr}(AC) \).

4. The first inequality \( 0 \leq \text{tr}(AB) \) can be obtained by (2). We can get the second inequality by (3) as follows:

\( \text{tr}(AB) \leq \text{tr}(A'B') \) and \( \text{tr}(A'B') \leq \text{tr}(AB) \leq \text{tr}(A'B') \).

□
Now let's compare these trace inequalities (2)-(4) to corresponding basic inequalities for real numbers as follows:

Inequality (2): this inequality is the counterpart of the inequality for real numbers:
if \( a \geq 0 \) and \( b \geq 0 \), then \( ab \geq 0 \). Note that for Hermitian operators \( A \) and \( B \) satisfying \( A \geq 0 \) and \( B \geq 0 \), we cannot definitely get \( AB \geq 0 \). This is because we even cannot ensure \( AB \) is a Hermitian operator, let alone it is a positive operator. For instance, set operator \( A = \ket{0}\bra{0} \geq 0 \) and operator \( B = \ket{+}\bra{+} \geq 0 \)

where \( \ket{+} = \frac{1}{\sqrt{2}} (\ket{0} + \ket{1}) \). But the product \( AB = \ket{0}\bra{0}\ket{+}\bra{+} = \frac{1}{\sqrt{2}} \ket{0}\bra{+} \) is not a Hermitian operator since its adjoint is not itself. However we can see, when we take trace function to the product \( AB \), the corresponding inequality, i.e. inequality (2), holds:

\[
\text{tr}(AB) = \text{tr}(\ket{0}\bra{0}\ket{+}\bra{+}) = \text{tr}(\frac{1}{\sqrt{2}} \ket{0}\bra{+}) = \frac{1}{\sqrt{2}} \bra{0}\ket{+} = \frac{1}{2} \geq 0 .
\]

Inequality (3): this inequality is the counterpart of the inequality for real numbers:
if \( a \leq b \) and \( c \geq 0 \), then \( ac \leq bc \). Note that for Hermitian operators \( A \), \( B \), and \( C \) satisfying \( B \leq C \) and \( A \geq 0 \), we cannot definitely get \( BA \leq CA \). In fact, like the above discussion on Inequality (2), we even cannot ensure that both \( BA \) and \( CA \) are Hermitian operators in this case. For instance, set \( B = -\ket{1}\bra{1} \leq C = \ket{0}\bra{0} \), and \( A = \ket{+}\bra{+} \geq 0 \). Neither the product

\[
BA = (-\ket{1}\bra{1})\ket{+}\bra{+} = -\frac{1}{\sqrt{2}} \ket{1}\bra{+}
\]

nor the product

\[
CA = \ket{0}\bra{0}\ket{+}\bra{+} = \frac{1}{\sqrt{2}} \ket{0}\bra{+}
\]

is a Hermitian operator since neither of their adjoints is itself. However we can see, when we take trace function to these two products \( BA \) and \( CA \), the corresponding inequality, i.e. inequality (3), holds:

\[
\text{tr}(BA) = \text{tr}((-\ket{1}\bra{1})\ket{+}\bra{+}) = \text{tr}(-\frac{1}{\sqrt{2}} \ket{1}\bra{+}) = -\frac{1}{\sqrt{2}} \leq \text{tr}(CA) = \text{tr}(\ket{0}\bra{0}\ket{+}\bra{+})
\]

\[
= \text{tr}(\frac{1}{\sqrt{2}} \ket{0}\bra{+}) = \frac{1}{2} .
\]

Inequality (4): this inequality is the counterpart of the inequality for real numbers:
if $0 \leq a \leq b$ and $0 \leq a' \leq b'$, then $0 \leq aa' \leq bb'$. Note that again, for Hermitian operators $A$, $B$, $A'$ and $B'$ satisfying $0 \leq A \leq A'$ and $0 \leq B \leq B'$, we cannot definitely get $0 \leq AB \leq A'B'$. For instance, $0 \leq A = |0\rangle\langle 0| \leq A' = I$ and

$0 \leq B = |+\rangle\langle +| \leq B' = I$. But the product $AB = |0\rangle\langle 0||+\rangle\langle +| = \frac{1}{\sqrt{2}}|0\rangle\langle +|$ is not a Hermitian operator. However we can see, when we take trace function to these two products $AB$ and $A'B'$, the corresponding inequality, i.e. inequality (4), holds:

$0 \leq tr(AB) = tr(|0\rangle\langle 0||+\rangle\langle +|) = \frac{1}{2} \leq tr(A'B') = tr(I) = 2$.

Finally, we give two examples to show the application of these trace inequalities for Hermitian operators. Suppose both $Q$ and $S$ are positive operators, and $P$ is a projection operator. Thus $Q - S \leq Q$ and $0 \leq P \leq I$. By trace inequality (3) in Theorem 3.2.2, we get $tr(P(Q-S)) \leq tr(PQ) \leq tr(Q)$. Another example is that we can get $-1 \leq tr(\rho\sigma) \leq 1$ where $\rho$ is a density operator and $\sigma \in \{\sigma_x, \sigma_y, \sigma_z\}$ is one of the three Pauli operators. We can obtain this inequality by trace inequality (3) in Theorem 3.2.2 and the inequality $-I \leq \sigma \leq I$ which we have mentioned in Example 3.1.2.

4 Conclusion

In this paper, we have presented and proved the order relation and some trace inequalities of Hermitian operators by comparison with their counterparts of real numbers. We have shown that the order relation $\leq$ for Hermitian operators has reflexivity, transitivity and antisymmetry, but it has no comparability, which means that not every pair of Hermitian operators is comparable. Hence unlike real numbers, Hermitian operators are not well ordered and have a partial order rather than a total order. Additionally, the set of real numbers is closed under the multiplication operation, while the set of Hermitian operators is not. In other words, the product of any two real numbers is always a real number, but the product of two Hermitian operators may not be a Hermitian operator. Nevertheless, considering taking the trace function for the product of two Hermitian operators
instead of the product itself, real numbers and Hermitian operators exhibit some similar aspects once again, which are the trace inequalities for Hermitian operators in this article.

Acknowledgements. This work is supported in part by the Scientific Research Fund of the Education Department of Sichuan Province of China (No. 18ZB0135) and the Research Fund of Key Laboratory of Pattern Recognition and Intelligent Information Processing of Sichuan Province in Chengdu University (No. MSSB-2015-10).

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Received: October 18, 2018; Published: November 5, 2018