Improvement of Uncertainty Relations for Mixed States

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Abstract

We study a possible improvement of uncertainty relations. The Heisenberg uncertainty relation employs commutator of a pair of conjugate observables to set the limit of quantum measurement of the observables. The Schrödinger uncertainty relation improves the Heisenberg uncertainty relation by adding the correlation in terms of anti-commutator. However both relations are insensitive whether the state used is pure or mixed. We improve the uncertainty relations by introducing additional terms which measure the mixtureness of the state. For the momentum and position operators as conjugate observables and for the thermal state of quantum harmonic oscillator, it turns out that the equalities in the improved uncertainty relations hold.

1 Introduction

Soon after Heisenberg and Schrödinger invented Quantum mechanics around 1925, Heisenberg discovered the uncertainty relation in 1927 [Hei]. The standard form of Heisenberg’s uncertainty relation for any pair of observables $A$ and $B$ and a density matrix $\rho$ is expressed as

$$\frac{1}{4} |\langle [A, B] \rangle_\rho|^2 \leq Var_\rho(A)Var_\rho(B),$$

(1.1)

where $Var_\rho(A) = tr(\rho A^2) - (tr(\rho A))^2$ is the variance of $A$ in the state defined by $\rho$, and $Var_\rho(B)$ is defined analogously, $\langle [A, B] \rangle_\rho = tr(\rho [A, B])$ is the expectation of the commutator $[A, B] = AB - BA$. The relation (1.1) states the fundamental limitation on quantum measurement for incompatible (non-commuting) observables and has been played fundamental role in quantum theory.
In 1930, Schrödinger improved the uncertainty relation (1.1) by including the correlation between observables:

\[
\frac{1}{4}|[\langle A, B \rangle]_{\rho}|^2 + \frac{1}{4}|\langle \{A_0, B_0\} \rangle|_{\rho}|^2 \leq \text{Var}_{\rho}(A)\text{Var}_{\rho}(B),
\]

where \( \langle \{A_0, B_0\} \rangle_{\rho} \) denotes the expectation of anti-commutator \( \{A_0, B_0\} = A_0B_0 + B_0A_0 \) and \( A_0 = A - \langle A \rangle_{\rho}, \ B_0 = B - \langle B \rangle_{\rho} \). The first term in the left hand side of (1.2) encodes incompatibility, while the second term encodes correlation between observables \( A \) and \( B \).

In recent years in the field of quantum computation and quantum information, the strong correlation, such as the phenomenon of entanglement, in the quantum world that can not be occurred in classical mechanics, has intensively studied [NC]. Thus one expects that the Schrödinger uncertainty relation will be played an important role in quantum theory [Suk].

In this paper, we improved the uncertainty relations (1.1) and (1.2) by introducing additional terms in the lower bounds of (1.1) and (1.2) respectively. We will show that for any observables \( A \) and \( B \), and any density matrix \( \rho \), the following uncertainty relations hold:

\[
\frac{1}{4}|[\langle A, B \rangle]_{\rho}|^2 + tr(A_0\rho^{1/2}A_0\rho^{1/2})(tr(B_0\rho^{1/2}B_0\rho^{1/2})) \leq \text{Var}_{\rho}(A)\text{Var}_{\rho}(B),
\]

and

\[
\frac{1}{4}|[\langle A, B \rangle]_{\rho}|^2 + \frac{1}{4}|\langle \{A_0, B_0\} \rangle|_{\rho}|^2 + M(A_0, B_0; \rho) \leq \text{Var}_{\rho}(A)\text{Var}_{\rho}(B),
\]

where the quantity \( M(A_0, B_0; \rho) \) is defined in Theorem 2.2 explicitly. Notice that the relation (1.3) and (1.4) are improved version of the relation (1.1) and (1.2) respectively. If the density matrix \( \rho \) is pure, the the second term in the left hand side of (1.3) and the third term in (1.4) are vanished and so (1.3) and (1.4) are reduced to the original relations (1.1) and (1.2) respectively.

It may be worth to mention that for any observable \( A \) the functional

\[ \rho \mapsto tr(A\rho^{1/4}A\rho^{1/4}) \]

is concave by Lieb’s concavity theorem [Lie], and so in a sense the values of additional terms in the above measure the mixtureness of \( \rho \). We also note that the Wigner-
Yanase skew information \([WY]\) is given by

\[
I(\rho, A) = -\frac{1}{2} \text{tr}(|\rho^{1/2}, A|^2) = \text{tr}(\rho A^2) - \text{tr}(A \rho^{1/2} A^{1/2})
\]

and so the terms we introduced are related to the Wigner-Yanase information. See Section 3 for the details.

In order to show that the uncertainty relation (1.3) and (1.4) are optimal in some special situations, we consider the position and momentum operators as a pair of conjugate observables in \(L^2(\mathbb{R})\), and choose the density operator \(\rho\) corresponding the thermal state (quasi-free state) for quantum harmonic oscillator. In this case, we show that the equalities in (1.3) and (1.4) hold. See Theorem 4.2.

Let us describe the main idea employed in this paper. Let \(A\) and \(B\) self-adjoint operators (observables) acting on a separable Hilbert space. Let \(\langle \cdot, \cdot \rangle\) be the Hilbert-Schmidt inner product defined on the class of Hilbert Schmidt operators:

\[
\langle A, B \rangle := \text{tr}(A^* B).
\]

Then the left hand side of (1.2) equals to \(\langle A_0 \rho^{1/2}, B_0 \rho^{1/2} \rangle^2\). In order to make \(\rho\) to play same role as \(A\) and \(B\), we introduce orthogonal decompositions

\[
A \rho^{1/2} = A_{\rho,+} + A_{\rho,-},
B \rho^{1/2} = B_{\rho,+} + B_{\rho,-}
\]

where

\[
A_{\rho,+} := \frac{1}{2}(A \rho^{1/2} + \rho^{1/2} A),
A_{\rho,-} := \frac{1}{2}(A \rho^{1/2} - \rho^{1/2} A),
\]

and \(B_{\rho,+}\) and \(B_{\rho,-}\) are defined analogously. Notice that \(\langle A_{\rho,-}, A_{\rho,+} \rangle = 0\) and \(\langle B_{\rho,-}, B_{\rho,+} \rangle = 0\). One observes that

\[
|\langle A_{\rho,+}, B_{\rho,-} \rangle| = |\langle A_{\rho,-}, B_{\rho,+} \rangle| = \frac{1}{4} |\langle [A, B] \rangle\|\rho|,
\]

The relation (1.3) will be followed from the above relation and the Schwarz inequality. See the proof of Theorem 2.1 in Section 3. The proof of (1.4) is a little complicate. Let \(S\) be the subspace spanned by \(B_{\rho,+}\) and \(B_{\rho,-}\) and let \(P_S\) be
the projection onto $S$. Denote by $\| \cdot \|_2$ the norm induced by $\langle \cdot, \cdot \rangle$. Notice that $\| P_S A \rho^{1/2} \|_2 \leq \| A \rho^{1/2} \|_2$. We will estimate $\| P_S A \rho \|_2$ to prove the relation (1.4). See Section 3 for the details.

There has been several proposes to quantify uncertainty by many authors. A prominent one is the Shannon entropy [BM, FS], and another one is the Fisher information arising in Statistical inference [Hal, Luo]. Recently Luo and Zhang [LZ] tried to characterize uncertainty relations by the Wigner-Yanase skew information [WY].

The paper is organized as follows: In Section 2, we list our main results, Theorem 2.1 and Theorem 2.2. In Section 3, we produce the proofs of main theorems by introducing the concept of orthogonal decompositions of $A\rho^{1/2}$ and $B\rho^{1/2}$. In Section 4, we give a brief discussion on possible optimal improvement. Then, we give an example of a mixed state (and a pair of conjugate observables) for which the equalities in (1.3) and (1.4) hold.

## 2 Improvement of Uncertainty Relations : Main Results

In this section we first list our main results, Theorem 2.1 and Theorem 2.2 and then give some remarks on the content of the results.

Let $\mathcal{H}$ be a separable Hilbert space. Denote by $\mathcal{L}(\mathcal{H})$ the algebra of all bounded linear operators on $\mathcal{H}$. An operator $T \in \mathcal{L}(\mathcal{H})$ is called Hilbert-Schmidt if $tr(T^*T) < \infty$, where $tr(T^*T)$ is the trace of $T^*T$. The class of all Hilbert-Schmidt operators is denoted by $\mathcal{L}_2(\mathcal{H})$.

We consider a pair of self-adjoint operators $A$ and $B$ acting on $\mathcal{H}$. Denote by $D(A)$ (resp. $D(B)$) the domain of $A$ (resp. $B$). Let $\rho$ be a density matrix (operator) on $\mathcal{H}$ ; $\rho \geq 0$ and $tr(\rho) = 1$. In order to care of the domain problems arising from the unboundedness of $A$ and $B$, we assume that the properties in the following assumption hold:

**Assumption 2.1** Let $A$ and $B$ be self-adjoint operators acting on a separable Hilbert space $\mathcal{H}$ and let $\rho \in \mathcal{L}(\mathcal{H})$ be a density matrix. We assume that the following properties hold:

(a) The inclusions $\rho^{1/2} \mathcal{H} \subset (D(A) \cap D(B))$, $A \rho^{1/2} \mathcal{H} \subset (D(A) \cap D(B))$ and $B \rho^{1/2} \mathcal{H} \subset (D(A) \cap D(B))$ hold.
(b) The composition maps $A\rho^{1/2}, B\rho^{1/2}, BA\rho^{1/2}, AB\rho^{1/2}, A^2\rho^{1/2}$ and $B^2\rho^{1/2}$ define Hilbert-Schmidt operators on $\mathcal{H}$.

(c) There is a dense set $D \subset (D(A) \cap D(B))$ such that the following inclusion hold: $AD \subset (D(A) \cap D(B))$ and $BD \subset (D(A) \cap D(B))$.

(d) The composition maps $\rho^{1/2}A, \rho^{1/2}B, \rho^{1/2}AB, \rho^{1/2}BA, \rho^{1/2}A^2$ and $\rho^{1/2}B^2$ are bounded on $D$. The bounded extensions of those operators, denoted by same symbols, are Hilbert-Schmidt.

We now list our main results. For notational simplicity, put

$$\langle T \rangle_\rho := tr(T\rho), \quad \|T\|_\rho^2 = tr(T^*T\rho)$$

for any (unbounded) operator, whenever the expressions in the above are well defined. Let $[A, B] := AB - BA$ and $\{A, B\} := AB + BA$ be the commutator and anti-commutator of $A$ and $B$ respectively. The following results are improved versions of the uncertainty relations (1.1) and (1.2):

**Theorem 2.1** Let $A$ and $B$ be self-adjoint operators acting on a separable Hilbert space $\mathcal{H}$ and let $\rho$ be a density matrix. Under Assumption 2.1, the relation

$$\frac{1}{4}(|\langle [A, B] \rangle_\rho|)^2 + tr(A\rho^{1/2}A\rho^{1/2})tr(B\rho^{1/2}B\rho^{1/2}) \leq \|A\|_\rho^2\|B\|_\rho^2$$

holds.

**Theorem 2.2** Let $A, B$ and $\rho$ be the operators as in Theorem 2.1. Under Assumption 2.1, the relation

$$\frac{1}{4}(|\langle [A, B] \rangle_\rho|)^2 + \frac{1}{4}(|\langle \{A, B\} \rangle_\rho|)^2 + M(A, B; \rho) \leq \|A\|_\rho^2\|B\|_\rho^2$$

holds, where $M(A, B; \rho) = \max\{M_1(A, B; \rho), M_1(B, A; \rho)\}$ and $M_1(A, B; \rho)$ is given by

$$M_1(A, B; \rho) := \frac{1}{4} (\frac{|\langle [A, B] \rangle_\rho|}{\|B\|_\rho^4} tr(B\rho^{1/2}B\rho^{1/2}))^2$$

if $tr(B\rho^{1/2}B\rho^{1/2}) < \|B\|_\rho^2$, and $M_1(A, B; \rho) = 0$ otherwise.
Under Assumption 2.1, one can check that each term in the relations (2.1) and (2.2) is well defined. It may be possible to weaken Assumption 2.1 to get the relations (2.1) and (2.2). Put

\[ A_0 := A - \langle A \rangle_0, \quad B_0 := B - \langle B \rangle_\rho. \]

If one replace \( A \) and \( B \) by \( A_0 \) and \( B_0 \) in the relations (2.1) and (2.2), one can see that Theorem 2.1 and Theorem 2.2 are improvements of Heisenberg’s uncertainty relation (1.1) and Schrödinger’s uncertainty relation (1.2) respectively. Notice that if \( \rho \) is pure, \( \text{tr}(A_0 \rho^{1/2} A_0 \rho^{1/2}) = \text{tr}(B_0 \rho^{1/2} B_0 \rho^{1/2}) = 0 \), and so the relations (2.1) and (2.2) are reduced to the relations (1.1) and (1.2) respectively for any pure states.

It may be worth to give discussions on the content of Theorem 2.1 and Theorem 2.2 in more details.

**Remark 2.1**

(a) As mentioned in Introduction, the functional

\[ \rho \mapsto \text{tr}(K \rho^t K^* \rho^{1-t}) \]

is concave for every \( 0 < t < 1 \) and \( K \in \mathcal{L}(\mathcal{H}) \) by Lieb’s concavity theorem [Lie]. Thus the values of the second term in l.h.s. of (2.1) and the third term in l.h.s. of (2.2) measure the mixtureness of the state. In addition, if it can be shown that the above functional increases as the mixtureness of \( \rho \) increases in the sense of Uhlmann [AU, OP], then obviously the additional terms in (2.1) and (2.2) increases as the mixtureness of \( \rho \) increases. However we do not know it yet.

(b) The Wigner-Yanase skew information [WY] for any observable \( A \) and a density matrix \( \rho \) is defined by

\[ I(\rho, A) := \frac{1}{2} \text{tr}([\rho^{1/2}, A][A, \rho^{1/2}]) \]

\[ = \text{tr}(A^2 \rho) - \text{tr}(A \rho^{1/2} A \rho^{1/2}). \]  

Thus the terms we introduced in Theorem 2.1 and Theorem 2.2 are related to the above skew information. Since \( 0 \leq I(\rho, A) \), we see that \( \text{tr}(A \rho^{1/2} A \rho^{1/2}) \leq \|A\|_\rho^2 \) and the equality holds if and only if \( [\rho, A] = 0 \). If \( \rho \) commutes with either \( A \) or else \( B \), then \( \langle [A, B] \rangle_\rho = 0 \). Thus, if \( A \) and \( B \) are conjugate observables, there does not exist such density matrix, and the strict inequalities \( \text{tr}(A \rho^{1/2} A \rho^{1/2}) < \|A\|_\rho^2 \) and \( \text{tr}(B \rho^{1/2} B \rho^{1/2}) < \|B\|_\rho^2 \) hold for any conjugate observables \( A \) and \( B \).
Remark 2.2 The inequality (2.2) is not optimal. In fact, we discarded complicated non-negative terms in the derivation of (2.2). We will give a discussion on the optimal lower bound of (2.2). See Theorem 4.1 in Section 4.

Remark 2.3 As an application of the uncertainty relations (2.1) and (2.2), we considered the position and momentum operators on $L^2(\mathbb{R})$ as a pair of conjugate observables and the density matrix $\rho$ corresponding to the thermal state for quantum harmonic oscillator. We proved that the equalities in the uncertainty relations in (2.1) and (2.2) hold in this case. See Theorem 4.2.

3 Proofs of Theorem 2.1 and Theorem 2.2

We produce the proofs of Theorem 2.1 and Theorem 2.2 in this Section. Let $A$ and $B$ self-adjoint operators and $\rho$ a density matrix satisfying the properties in Assumption 2.1. For notational brevity, we write

$$A_\rho := A\rho^{1/2}, \quad B_\rho := B\rho^{1/2}. \tag{3.1}$$

We decompose $A_\rho$ and $B_\rho$ as

$$A_\rho = A_{\rho,+} + A_{\rho,-},$$
$$B_\rho = B_{\rho,+} + B_{\rho,-}, \tag{3.2}$$

where

$$A_{\rho,+} := \frac{1}{2} (A\rho^{1/2} + \rho^{1/2}A) = \frac{1}{2} \{A, \rho^{1/2}\},$$
$$A_{\rho,-} := \frac{1}{2} (A\rho^{1/2} - \rho^{1/2}A) = \frac{1}{2} [A, \rho^{1/2}], \tag{3.3}$$
$$B_{\rho,+} := \frac{1}{2} (B\rho^{1/2} + \rho^{1/2}B) = \frac{1}{2} \{B, \rho^{1/2}\},$$
$$B_{\rho,-} := \frac{1}{2} (B\rho^{1/2} - \rho^{1/2}B) = \frac{1}{2} [B, \rho^{1/2}].$$

Denote by $\langle T, S \rangle, T, S \in \mathcal{L}_2(\mathcal{H})$, the Hilbert-Schmidt inner product on $\mathcal{L}_2(\mathcal{H})$:

$$\langle T, S \rangle := \text{tr}(T^*S), \quad \forall T, S \in \mathcal{L}_2(\mathcal{H}), \tag{3.4}$$

and $\|T\|_2$ the induced norm:

$$\|T\|_2^2 := \text{tr}(T^*T). \tag{3.5}$$

Here we have used the norm $\|T\|_2$ to distinguish it from the operator norm $\|T\|$. In the sequel, we assume that the properties in Assumption 2.1 hold.
Lemma 3.1  
(a) \((A\rho^{1/2})^* = \rho^{1/2}A\) and \((B\rho^{1/2})^* = \rho^{1/2}B\).

(b) The equalities
\[ \rho^{1/2}(A^2\rho^{1/2}) = (\rho^{1/2}A)(A\rho^{1/2}), \quad \rho^{1/2}(B^2\rho^{1/2}) = (\rho^{1/2}B)(B\rho^{1/2}), \]
\[ \rho^{1/2}(AB\rho^{1/2}) = (\rho^{1/2}A)(B\rho^{1/2}), \quad \rho^{1/2}(BA\rho^{1/2}) = (\rho^{1/2}B)(A\rho^{1/2}) \]
hold, where \(\rho^{1/2}(A^2\rho^{1/2})\) is the composite map (operator product) of \(\rho^{1/2}\) and \(A^2\rho^{1/2}\), and \((\rho^{1/2}A)(A\rho^{1/2})\) the composite map of \(\rho^{1/2}A\) and \(A\rho^{1/2}\), etc.

(c) \(\langle A_{\rho,+}, A_{\rho,-} \rangle = 0\) and \(\langle B_{\rho,+}, B_{\rho,-} \rangle = 0\).

Proof: (a) By Assumption 2.1(b)-(c), one has that for any \(\varphi \in D\) and \(\eta \in \mathcal{H}\)
\[ (\varphi, A\rho^{1/2}\eta) = (\rho^{1/2}A\varphi, \eta). \]
It follows from Assumption 2.1(d) that the above equality holds for any \(\varphi, \eta \in \mathcal{H}\) and so \((A\rho^{1/2})^* = \rho^{1/2}A\). The method used for \(A\rho^{1/2}\) yields \((B\rho^{1/2})^* = \rho^{1/2}B\).

(b) Those equalities follow from Assumption 2.1(b) and the part (a) of the Lemma.

(c) The part (c) of the Lemma follows from the definitions of \(A_{\rho,\pm}\) and \(B_{\rho,\pm}\) in (3.3) and the trace property; \(tr(TS) = tr(ST)\). □

It follows from Lemma 3.1(c) that the decompositions in (3.2) are orthogonal decompositions. Also Lemma 3.1(a) shows that \(A_{\rho,\pm}\) and \(B_{\rho,\pm}\) are self-adjoint, and \((A_{\rho,-})^* = -A_{\rho,-}\) and \((B_{\rho,-})^* = -B_{\rho,-}\).

Lemma 3.2 The equalities
\[ \langle A_{\rho,\pm}, A_{\rho,\pm} \rangle = \frac{1}{2}(tr(A^2\rho) \pm tr(A\rho^{1/2}A\rho^{1/2})), \]
\[ \langle B_{\rho,\pm}, B_{\rho,\pm} \rangle = \frac{1}{2}(tr(B^2\rho) \pm tr(B\rho^{1/2}B\rho^{1/2})), \]
\[ \langle B_{\rho,\pm}, A_{\rho,\pm} \rangle = \frac{1}{4}(tr([A, B]\rho) \pm 2tr(B\rho^{1/2}A\rho^{1/2})), \]
\[ \langle B_{\rho,\pm}, A_{\rho,\mp} \rangle = \frac{1}{4}(tr([B, A]\rho) \pm 2tr(A\rho^{1/2}B\rho^{1/2})), \]
hold.

Proof: The equalities follows from the definitions of \(A_{\pm}\) and \(B_{\pm}\) in (3.3) and direct computations. □

Notice that by the first and second equalities in Lemma 3.2 one has that
\[ \|A_{\rho, \pm}\|_2^2 = \frac{1}{2}\{\|A\|_\rho^2 \pm \text{tr}(A\rho^{1/2}A\rho^{1/2})\}, \]
\[ \|B_{\rho, \pm}\|_2^2 = \frac{1}{2}\{\|B\|_\rho^2 \pm \text{tr}(B\rho^{1/2}B\rho^{1/2})\}. \]  

(3.6)

Also one recognizes that the Wigner-Yanase skew information \( I(\rho, A) \) and \( \|A_{\rho, -}\| \) are related by
\[ I(\rho, A) = 2\|A_{\rho, -}\|^2. \]  

(3.7)

See the definition of \( I(\rho, A) \) in (2.4).

We are now ready to prove Theorem 2.1 and Theorem 2.2. It follows from (3.1) that
\[ \langle B_{\rho}, A_{\rho} \rangle = \text{tr}(BA\rho) = \frac{1}{2}\text{tr}(\{B, A\}\rho) + \frac{1}{2}\text{tr}(\{B, A\}\rho). \]

Since the first term in the r.h.s. of the above is real and the second term is pure imaginary,
\[ |\langle B_{\rho}, A_{\rho} \rangle|^2 = \frac{1}{4}|\text{tr}(\{B, A\}\rho)|^2 + \frac{1}{4}|\text{tr}(\{B, A\}\rho)|^2, \]  

(3.8)

and so by the Schwarz inequality, the Schrödinger uncertainty relation
\[ \frac{1}{4}(\text{tr}(\{B, A\}\rho)|^2 + \frac{1}{4}|\text{tr}(\{B, A\}\rho)|^2 \leq \|A\|_\rho^2\|B\|_\rho^2 \]  

(3.9)

holds. Recall that \( \|A\|_\rho^2 = \|A\|_{\rho, -}^2 \) and \( \|B\|_\rho^2 = \|B\|_{\rho, +}^2 \).

Proof of Theorem 2.1. It follows from the Schwarz inequality and (3.6) that
\[ |\langle B_{\rho, +}, A_{\rho, -} \rangle|^2 \leq \|B_{\rho, +}\|_2^2 \|A_{\rho, -}\|_2^2 \]
\[ = \frac{1}{4}(\|B\|_\rho^2 + \text{tr}(B\rho^{1/2}A\rho^{1/2}))\|A\|_\rho^2 - \text{tr}(A\rho^{1/2}A\rho^{1/2})), \]
\[ |\langle B_{\rho, -}, A_{\rho, +} \rangle|^2 \leq \|B_{\rho, -}\|_2^2 \|A_{\rho, +}\|_2^2 \]
\[ = \frac{1}{4}(\|B\|_\rho^2 - \text{tr}(B\rho^{1/2}A\rho^{1/2}))\|A\|_\rho^2 + \text{tr}(A\rho^{1/2}A\rho^{1/2})). \]

Thus, by the fourth equality in Lemma 3.2 and the above inequality, we have
\[ \frac{1}{8}|\text{tr}(\{B, A\}\rho)|^2 = |\langle B_{\rho, +}, A_{\rho, -} \rangle|^2 + |\langle B_{\rho, -}, A_{\rho, +} \rangle|^2 \]
\[ \leq \frac{1}{2}\{\|B\|_\rho^2\|A\|_\rho^2 - \text{tr}(B\rho^{1/2}B\rho^{1/2})\text{tr}(A\rho^{1/2}A\rho^{1/2})). \]

The above relation equals to that in Theorem 2.1. □.

Now, let us turn to the proof of Theorem 2.2. Recall that the class \( \mathcal{L}_2(\mathcal{H}) \) of all Hilbert-Schmidt operator is a Hilbert space with the Hilbert-Schmidt inner product
\langle \cdot, \cdot \rangle$ defined in (3.4). Denote by $\hat{A}_{\rho, \pm}$ and $\hat{B}_{\rho, \pm}$ the normalized vectors in $L^2(H)$ in the direction of $A_{\rho, \pm}$ and $B_{\rho, \pm}$ respectively:

$$\hat{A}_{\rho, \pm} = A_{\rho, \pm} / \|A_{\rho, \pm}\|_2, \quad \hat{B}_{\rho, \pm} = B_{\rho, \pm} / \|B_{\rho, \pm}\|_2.$$ 

(3.10)

If $\|A_{\rho, \pm}\|_2 = 0$ (resp. $\|B_{\rho, \pm}\|_2 = 0$), we set $\hat{A}_{\rho, \pm} = 0$ (resp. $\hat{B}_{\rho, \pm} = 0$). By (3.2) and (3.10),

$$A_{\rho} = \|A_{\rho, +}\|_2 \hat{A}_{\rho, +} + \|A_{\rho, -}\|_2 \hat{A}_{\rho, -},$$

$$B_{\rho} = \|B_{\rho, +}\|_2 \hat{B}_{\rho, +} + \|B_{\rho, -}\|_2 \hat{B}_{\rho, -}. \quad \text{(3.11)}$$

We introduce vectors orthogonal to $A_{\rho}$ and $B_{\rho}$ by

$$A_{\rho}^\perp = \|A_{\rho, -}\|_2 \hat{A}_{\rho, +} - \|A_{\rho, +}\|_2 \hat{A}_{\rho, -},$$

$$B_{\rho}^\perp = \|B_{\rho, -}\|_2 \hat{B}_{\rho, +} - \|B_{\rho, +}\|_2 \hat{B}_{\rho, -}. \quad \text{(3.12)}$$

It is easy to check that

$$\|A_{\rho}^\perp\|_2 = \|A_{\rho}\|_2, \quad \|B_{\rho}^\perp\|_2 = \|B_{\rho}\|_2,$$

$$\langle A_{\rho}^\perp, A_{\rho} \rangle = 0, \quad \langle B_{\rho}^\perp, B_{\rho} \rangle = 0. \quad \text{(3.13)}$$

Denote by $\tilde{S}$ and $S$ the subspace of $L^2(H)$ spanned by $\{\hat{A}_{\rho, +}, \hat{A}_{\rho, -}\}$ and $\{\hat{B}_{\rho, +}, \hat{B}_{\rho, -}\}$ respectively, and let $P_S$ be the projection to $S$.

**Proposition 3.1** The inequality

$$|\langle B_{\rho}, A_{\rho} \rangle|^2 + |\langle B_{\rho}^\perp, A_{\rho} \rangle|^2 \leq \|B_{\rho}\|_2^2 \|A_{\rho}\|_2^2$$

holds.

**Proof:** Let $\hat{B}_{\rho}$ and $\hat{B}_{\rho}^\perp$ be normalized vectors in the directions of $B_{\rho}$ and $B_{\rho}^\perp$ respectively:

$$\hat{B}_{\rho} = B_{\rho} / \|B_{\rho}\|_2, \quad \hat{B}_{\rho}^\perp = B_{\rho}^\perp / \|B_{\rho}\|_2.$$ 

Since $\{\hat{B}_{\rho}, \hat{B}_{\rho}^\perp\}$ is an orthonormal basis of $S$, we have

$$\|P_S A_{\rho}\|^2 = |\langle \hat{B}_{\rho}, P_S A_{\rho} \rangle|^2 + |\langle \hat{B}_{\rho}^\perp, P_S A_{\rho} \rangle|^2 \quad \text{(3.14)}$$

and so

$$|\langle \hat{B}_{\rho}, A_{\rho} \rangle|^2 + |\langle \hat{B}_{\rho}^\perp, A_{\rho} \rangle|^2 = \|P_S A_{\rho}\|^2 \leq \|A_{\rho}\|_2^2.$$ 

By multiplying $\|B_{\rho}\|_2^2$ to the both sides of the above inequality, we proved the lemma.

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Lemma 3.3 The equality

$$|\langle B^\perp_\rho, A \rangle|^2 = M_1(A, B; \rho) + M_2(A, B; \rho),$$

holds, where $M_1(A, B; \rho)$ is given by (2.3) in Theorem 2.2 and

$$M_2(A, B; \rho) = \frac{1}{4} (\|B_{\rho+,\rho^-}\|^2 \|B_{\rho-,\rho^+}\|^2)^{-1} \left[ \|B\|^2 \text{tr}(B^{1/2}B\rho^{-1/2}) - \frac{1}{2} \langle \{B, A\}\rangle \text{tr}(B^{1/2}B\rho^{1/2}) \right]^2$$

if $\text{tr}(B^{1/2}B\rho^{1/2}) < \|B\|^2$, and $M_2(A, B; \rho) = 0$ otherwise.

Proof: By the definition of $B^\perp_\rho$ in (3.12),

$$\langle B^\perp_\rho, A \rangle = \langle \|B_{\rho-,\rho^+}\|^2 \hat{B}_{\rho-,\rho^+} - \|B_{\rho+,\rho^-}\|^2 \hat{B}_{\rho+,\rho^-}, A_{\rho+,\rho^-} \rangle$$

$$= \left\{ \frac{\|B_{\rho-,\rho^+}\|^2}{\|B_{\rho+,\rho^-}\|^2} \langle B_{\rho+,\rho^-}, A_{\rho+,\rho^-} \rangle - \frac{\|B_{\rho+,\rho^+}\|^2}{\|B_{\rho-,\rho^-}\|^2} \langle B_{\rho-,\rho^+}, A_{\rho-,\rho^+} \rangle \right\}$$

$$+ \left\{ \frac{\|B_{\rho+,\rho^+}\|^2}{\|B_{\rho-,\rho^-}\|^2} \langle B_{\rho-,\rho^+}, A_{\rho+,\rho^+} \rangle - \frac{\|B_{\rho-,\rho^-}\|^2}{\|B_{\rho+,\rho^+}\|^2} \langle B_{\rho+,\rho^+}, A_{\rho-,\rho^-} \rangle \right\}.$$

Since the first term in r.h.s. of the last equality in the above is real and the second term is pure imaginary, we have

$$|\langle B^\perp_\rho, A \rangle|^2 = M_1(A, B; \rho) + M_2(A, B; \rho),$$

where

$$M_1(A, B; \rho) = \left[ \frac{\|B_{\rho-,\rho^+}\|^2}{\|B_{\rho+,\rho^-}\|^2} \langle B_{\rho+,\rho^-}, A_{\rho+,\rho^-} \rangle - \frac{\|B_{\rho+,\rho^+}\|^2}{\|B_{\rho-,\rho^-}\|^2} \langle B_{\rho-,\rho^+}, A_{\rho-,\rho^+} \rangle \right]^2,$$

$$M_2(A, B; \rho) = \left[ \frac{\|B_{\rho+,\rho^+}\|^2}{\|B_{\rho-,\rho^-}\|^2} \langle B_{\rho-,\rho^+}, A_{\rho+,\rho^+} \rangle - \frac{\|B_{\rho-,\rho^-}\|^2}{\|B_{\rho+,\rho^+}\|^2} \langle B_{\rho+,\rho^+}, A_{\rho-,\rho^-} \rangle \right]^2.$$

By Lemma 3.2

$$M_1(A, B; \rho) = \frac{1}{4^2} |\langle [B, A] \rangle |^2 (\|B_{\rho+,\rho^-}\|^2 \|B_{\rho-,\rho^+}\|^2)^{-2} (\|B_{\rho-,\rho^-}\|^2 - \|B_{\rho+,\rho^+}\|^2)^2,$$

Substituting (3.10) into the above expression, we proved that $M_1(A, B; \rho)$ in the above equals to that in (2.3).

Next, we consider $M_2(A, B; \rho)$ in (3.16). $M_2(A, B; \rho)$ can be expressed as

$$M_2(A, B; \rho) = (\|B_{\rho+,\rho^-}\|^2 \|B_{\rho-,\rho^+}\|^2)^{-2} \left[ \|B_{\rho-,\rho^+}\|^2 \langle B_{\rho+,\rho^-}, B_{\rho-,\rho^+} \rangle - \|B_{\rho+,\rho^+}\|^2 \langle B_{\rho-,\rho^+}, A_{\rho-,\rho^+} \rangle \right]^2.$$
Using Lemma 3.2 and (3.6), one can check that the above expression equals to that in (3.15). Notice that, if \( \| B_{\rho,-} \|_2 = 0 \), then \( B_{\rho} = 0 \) by (3.12). Thus \( M_1(A, B; \rho) = M_2(A, B; \rho) = 0 \) in this case. This proved the lemma completely. \( \square \)

Proof of Theorem 2.2. Since \( M_2(A, B; \rho) \geq 0 \), Theorem 2.2 for \( M_1(A, B; \rho) \) follows from Proposition 3.1, (3.8) and Lemma 3.3. By interchanging the role of \( A_{\rho} \) and \( B_{\rho} \), we proved the theorem completely. \( \square \).

4 Optimal Improvement and Application

We give a brief discussion on the optimal improvement of Theorem 2.2 which can be obtained by the method used in Section 3. Then, as an application of Theorem 2.1 and Theorem 2.2, we consider the thermal states of quantum harmonic oscillator.

4.1 Possible Optimal Improvement

Recall that \( S \) is the subspace of \( \mathcal{L}_2(\mathcal{H}) \) spanned by \( \{ \hat{B}_{\rho,+}, \hat{B}_{\rho,-} \} \) and \( P_S \) is the projection onto \( S \). In the proof of Theorem 2.2, we have used the identity (3.14). The quantity \( \| P_S A_{\rho} \| \) is the length of the projection of \( A_{\rho} \) onto \( S \). Thus it is clear that, in order to obtain the optimal improvement one has to find the vector \( X \) with \( \| X \|_2 = \| A_{\rho} \|_2 \) in the subspace \( \tilde{S} \) spanned by \( \{ \hat{A}_{\rho,+}, \hat{A}_{\rho,-} \} \), which has the biggest component in \( S \).

In order to find such a vector in \( \tilde{S} \), put

\[
X = \alpha A_{\rho} + \beta A_{\rho}^\perp,
\]

where \( \alpha \) and \( \beta \) are complex constants satisfying

\[
|\alpha|^2 + |\beta|^2 = 1
\]

One has that

\[
\| P_S X \|_2^2 = \alpha^2 \| P_S A_{\rho} \|_2^2 + \bar{\alpha} \beta \langle P_S A_{\rho}, P_S A_{\rho}^\perp \rangle + \alpha \bar{\beta} \langle P_S A_{\rho}^\perp, P_S A_{\rho} \rangle + |\beta|^2 \| P_S A_{\rho}^\perp \|_2^2.
\]

One can choose \( \alpha \) such that \( \alpha \geq 0 \). The first and last terms in r.h.s. of the above are non-negative. To make the other terms non-negative, we choose \( \beta \) as

\[
\beta = \gamma \langle P_S A_{\rho}^\perp, P_S A_{\rho} \rangle / |\langle P_S A_{\rho}^\perp, P_S A_{\rho} \rangle|,
\]

where

\[
\gamma = \left( \frac{\| P_S A_{\rho}^\perp \|_2^2}{\| P_S A_{\rho} \|_2^2} \right)^{\frac{1}{2}}.
\]
where $\gamma \geq 0$. We then have

$$\|P_SX\|_2^2 = \alpha^2\|P_SA_\rho\|_2^2 + 2\alpha\gamma|\langle P_SA_\rho, P_SA_\perp\rangle| + \gamma^2\|P_SA_\perp\|_2^2, \quad (4.1)$$

where $\alpha$ and $\gamma$ are non-negative real numbers satisfying

$$\alpha^2 + \gamma^2 = 1. \quad (4.2)$$

Thus the problem is to maximize (4.1) under the constrain (4.2). The problem can be solved by the method of the Lagrange multiplier.

We use the following notation:

$$a = \|P_SA_\rho\|_2^2, \quad b = \|P_SA_\perp\|_2^2, \quad c = |\langle P_SA_\rho, P_SA_\perp\rangle|. \quad (4.3)$$

Put

$$d = (a - b)/2c. \quad (4.4)$$

The method of the Lagrange multiplier implies that

$$a\alpha + c\gamma = \lambda\alpha$$
$$b\gamma + c\alpha = \lambda\gamma,$$

where $\lambda$ is the Lagrange multiplier. The above relations imply

$$\alpha^2 - 2d\alpha\gamma - \gamma^2 = 0. \quad (4.5)$$

Since $\alpha > 0$, one has that

$$\alpha = (d + \sqrt{d^2 + 1})\gamma. \quad (4.6)$$

From (4.2) and (4.6), $\alpha$ and $\gamma$ can be solved explicitly. One may check that

$$\gamma^2 = 1/(1 + (d + \sqrt{d^2 + 1})^2)$$
$$= 1/[2(d^2 + 1) + 2d\sqrt{d^2 + 1}]. \quad (4.7)$$

The relation (4.5) and (4.2) imply

$$\alpha\gamma = (1 - 2\gamma^2). \quad (4.8)$$

We substitute (4.7) and (4.8) into

$$\|P_SX\|_2^2 = a(1 - \gamma^2) + 2c\alpha\gamma + b\gamma^2$$
to obtain

\[ \| P_SX \|_2^2 = a + c(\sqrt{d^2 + 1} - d) \]

\[ = a + \frac{1}{2}\left\{[(a - b)^2 + 4c^2]^{1/2} - (a - b)\right\}. \tag{4.9} \]

We leave that detailed derivation of (4.9) to the reader.

Let us denote by

\[ m_3(A, B; \rho) := \frac{1}{2}\left\{[(a - b)^2 + 4c^2]^{1/2} - (a - b)\right\}, \tag{4.10} \]

where \( a, b \) and \( c \) are given by (4.3). Put

\[ M_3(A, B; \rho) := \| B \|_\rho^2 m_3(A, B; \rho). \tag{4.11} \]

We then above the following result:

**Theorem 4.1** The relation

\[ \frac{1}{4}|\langle [A, B] \rangle_\rho|^2 + \frac{1}{4}|\langle \{A, B\} \rangle_\rho|^2 + \tilde{M}(A, B; \rho) \leq \| A \|_\rho^2 \| B \|_\rho^2. \tag{4.12} \]

holds, where

\[ \tilde{M}(A, B; \rho) = \max\left\{ \sum_{k=1}^3 M_k(A, B; \rho), \sum_{k=1}^3 M_k(B, A; \rho)\right\}, \]

and \( M_1(A, B; \rho), M_2(A, B; \rho) \) and \( M_3(A, B; \rho) \) are given as in (2.3), (3.15) and (4.11) respectively.

**Proof:** It follows from (4.9) that

\[ \| B \|_\rho^2 \| P_SA \|_2^2 + M_3(A, B; \rho) = \| B \|_\rho^2 \| P_SX \|_2^2 \leq \| B \|_\rho^2 \| X \|_2^2 = \| B \|_\rho^2 \| A \|_\rho^2. \tag{4.12} \]

We recall from (3.14) and Lemma 3.3 that

\[ \| B \|_\rho^2 \| P_SA \|_2^2 = |\langle B, A \rangle_\rho|^2 + M_1(A, B; \rho) + M_2(A, B; \rho). \tag{4.13} \]

Thus the theorem follows from (4.12), (4.13) and (3.8) together with an interchanging the role of \( A \) and \( B \). \( \Box \)

Even if \( M_3(A, B; \rho) \) can be expressed explicitly in terms of \( \| A_{\rho,\pm} \|_2, \| B_{\rho,\pm} \|_2 \), etc, the expression is complicate and so we do not present it here.
4.2 An Application

In $L^2(\mathbb{R})$, the momentum operator $P$ and the position operator $Q$ are represented by

$$ P = i \frac{d}{dx}, \quad Q = x. \quad (4.14) $$

It is convenient to introduce the annihilation and creation operators which are defined as

$$ a = \frac{1}{\sqrt{2}} (x + \frac{d}{dx}), \quad a^\ast = \frac{1}{\sqrt{2}} (x - \frac{d}{dx}). $$

Those operators satisfy the canonical commutation relations

$$ [a, a^\ast] = 1, \quad [a, a] = [a, a^\ast] = 0, \quad (4.15) $$

and $P$ and $Q$ can be written as

$$ P = \frac{i}{\sqrt{2}} (a - a^\ast), \quad Q = \frac{1}{\sqrt{2}} (a + a^\ast). \quad (4.16) $$

Let $N$ be the number operator defined by

$$ N = a^\ast a. \quad (4.17) $$

The Hamiltonian for quantum harmonic oscillator is given by

$$ H = \frac{1}{2} (P^2 + Q^2) = N + \frac{1}{2}. \quad (4.18) $$

Let $\Omega$ be the ground state of $H$ and let $\mathcal{F}_0$ be the dense subset consisting of finite linear combinations of vectors $\{(a^\ast)^n \Omega, n \in \mathbb{N}\}$. Then $\mathcal{F}_0$ is a common core for $a, a^\ast$ and $N$. For the details, we refer to Section 5.2 of [BR].

The density operator $\rho$ corresponding to the thermal state is given by

$$ \rho = \frac{1}{Z} \exp(-\beta H) = \frac{1}{Z} \exp(\beta(N + \frac{1}{2})), \quad (4.19) $$

where $Z = tr(\exp(-\beta H))$ and $\beta > 0$ the inverse of the temperature.

**Theorem 4.2** Let $A = P$ and $B = Q$ and let $\rho$ be given by (4.19). Then the properties in Assumption 2.1 hold (with $D = \mathcal{F}_0$). Moreover each side of (2.1) and (2.2) equals to $\cosh^2(\beta/2))/4 \sinh^2(\beta/2)$, and so the equalities in the uncertainty relations in Theorem 2.1 and Theorem 2.2 hold.
Proof: Let $a_k^\#$, $k = 1, 2, \cdots, n$, be either $a^*$ or else $a$. It can be checked that

$$\| \prod_{k=1}^n a_k^\# \varphi \| \leq \| (N + n + 1)^{n/2} \varphi \|$$

for any $\varphi \in \mathcal{F}_0$. Thus $(\prod_{k=1}^n a_k^\#)(N + n + 1)^{-n/2}$ is bounded operator for each $n$. Thus the properties (a) and (b) in Assumption 2.1 hold.

Notice that the equalities

$$a(N + 1) = (N + 2)a, \quad a^*(N + 2) = (N + 1)a^*$$

hold on $\mathcal{F}_0$. The above equalities imply

$$(N + 2)^{-1}a = a(N + 1)^{-1}, \quad (N + 1)^{-1}a^* = a^*(N + 2)^{-1}.$$ 

Using the above relations repeatedly, one can check that the properties (c) and (d) in Assumption 2.1 hold. We leave the details to the reader.

Next, we compute each side of (2.1) and (2.2). A direct computation shows that

$$\langle a^* a \rangle_\rho = e^{-\beta} / (1 - e^{-\beta}). \quad (4.20)$$

It follows from (4.20) and the canonical commutation relations (4.15) that

$$\| Q \|_\rho^2 = \frac{1}{2} tr((a + a^*)(a + a^*)\rho) = \frac{1}{2} + e^{-\beta} / (1 - e^{-\beta}) = \frac{1}{2} \cosh(\beta/2) / \sinh(\beta/2). \quad (4.21)$$

The method used in the above gives

$$\| P \|_\rho^2 = \frac{1}{2} \cosh(\beta/2) / \sinh(\beta/2). \quad (4.22)$$

It can be checked that

$$\rho^{1/2}a = e^{\beta/2}a\rho^{1/2}, \quad \rho^{1/2}a^* = e^{-\beta/2}a^*\rho^{1/2}. \quad (4.23)$$

We use (4.23) to obtain

$$tr(Q\rho^{1/2}Q^{1/2}Q) = \frac{1}{2} tr((a + a^*)(e^{\beta/2}a + e^{-\beta/2}a^*)\rho) = \frac{1}{2} tr(e^{-\beta/2}aa^* + e^{\beta/2}a^*a) = 1/2 \{ e^{-\beta/2} + (e^{\beta/2} + e^{-\beta/2})e^{-\beta} / (1 - e^{-\beta}) \} = 1/2 \sinh(\beta/2), \quad (4.24)$$

$$tr(P\rho^{1/2}P^{1/2}P) = 1/2 \sinh(\beta/2). \quad (4.25)$$
A direct computation yields

\[ \langle \{ P, Q \} \rangle_\rho = 0, \quad tr(P \rho^{1/2} Q \rho^{1/2}) = 0. \]  \hspace{1cm} (4.26)

Thus (4.21) and (4.22) imply

\[ \| P \|_\rho^2 \| Q \|_\rho^2 = \cosh^2(\beta/2)/4 \sinh^2(\beta/2). \]  \hspace{1cm} (4.27)

Since \([ P, Q ] = i\), (4.21) and (4.24) imply that

\[ \text{l.h.s. of (2.1)} = \frac{1}{4} + \frac{1}{4 \sinh^2(\beta/2)} = \cosh^2(\beta/2)/4 \sinh^2(\beta/2). \]  \hspace{1cm} (4.28)

Next, we compute the l.h.s. of (2.2). We use (4.21) and (4.24) to obtain

\[ \| Q \|_\rho^4 - (tr(Q \rho^{1/2} Q \rho^{1/2}))^2 = \frac{1}{4} \left\{ \frac{\cosh^2(\beta/2)}{\sinh^2(\beta/2)} - \frac{1}{\sinh^2(\beta/2)} \right\} \]
\[ = \frac{1}{4}; \]

and so

\[ M_1(P, Q; \rho) = (tr(Q \rho^{1/2} Q \rho^{1/2}))^2 = 1/4 \sinh^2(\beta/2). \]

Thus we conclude that

\[ \text{l.h.s. of (2.2)} = \cosh^2(\beta/2)/4 \sinh^2(\beta/2). \]  \hspace{1cm} (4.29)

Combining (4.27) - (4.29), we complete the proof of Theorem 4.2. \( \Box \)

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