Abstract

The example of nonpositive trace-class Hermitian operator for which Robertson–Schrödinger uncertainty relation is fulfilled is presented. The partial scaling criterion of separability of multimode continuous variable system is discussed in the context of using nonpositive maps of density matrices.

DOES THE UNCERTAINTY RELATION DETERMINE THE QUANTUM STATE?

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1 Introduction

The main difference of quantum and classical mechanics is connected with the uncertainty relations by Heisenberg [1] and by Schrödinger [2] and Robertson [3]. The uncertainty relations were studied in [4] and [5]. A review of the uncertainty relations is presented in [6]. The uncertainty relation is used to formulate the separability criterion for composed system states. For continuous variables, the separability criterion based on Peres–Horodecki partial transpose of subsystem density matrix [7, 8] was applied in [9] to the case of two-mode system using the Schrödinger–Robertson uncertainty relation. The partial scaling transform was suggested as a separability criterion for multimode continuous-variable systems in [10] and the key role is in using the multimode Robertson uncertainty relation. A recent review is presented in [11].
In view of these applications, as well as due to the necessity of a deeper understanding the role of uncertainty relations in characterizing the set of all admissible quantum states. In this paper, we address in this paper to the following question.

Does the uncertainty-relation imply that the density state [12, 13] used to evaluate it is really Hermitian, trace-class and nonnegative? In other words, is the uncertainty-relation both a necessary and sufficient condition for the density state to be nonnegative?

The aim of this paper is to show that the uncertainty-relation fulfilling is necessary but not sufficient condition for the nonnegativity of the density matrix. We present the example of the ”pseudodensity operator” for which the uncertainty relation is fulfilled but the operator itself has negative eigenvalues.

The other goal of this paper is to discuss a possible role of nonpositive maps to detect the entanglement. We consider the two-mode and multimode Gaussian states applying the momentum scaling transform which turns out to be nonpositive. ¹ We show how nonpositive map of subsystem density matrix preserving the uncertainty relation can be used to formulate the separability criterion.

The paper is organized as follows.

In Section 2, we review the standard derivation of the Schrödinger–Robertson uncertainty relation. In Section 3, we describe the nonpositive map of density operator for continuous variables which is scaling transform of momentum in the Wigner-function representation of the quantum state. In Section 4, the example of Hermitian nonpositive operator with trace equal to unity for which the Schrödinger–Robertson uncertainty relation takes place is presented. In Section 5, we formulate a criterion of separability using nonpositive scaling map (and the other maps). The perspectives and conclusions are done in Section 6.

2 Schrödinger–Robertson uncertainty relation

In this section, we review the derivation of position–momentum uncertainty relation.

Given nonegative Hermitian operator ˆ which is the density operator of

¹E.V. Shchukin directed our attention to the nonpositivity of this map.
a quantum state with $\text{Tr} \hat{\rho} = 1$. The obvious relation holds
\[ \text{Tr} (\hat{F}^\dagger \hat{F} \hat{\rho}) \geq 0, \quad (1) \]
where $\hat{F}$ is an arbitrary operator.

Let us take operator $\hat{F}$ in the form
\[ \hat{F} = c_1 \hat{q} + c_2 \hat{p}, \quad (2) \]
where $\hat{q}$ and $\hat{p}$ are canonical position and momentum operators, e.g., for harmonic oscillator, and $c_1$ and $c_2$ are complex numbers.

We rewrite (2) in the form
\[ \hat{F} = 2 \sum_{\alpha=1}^{2} c_\alpha \hat{Q}_\alpha, \quad \hat{Q}_1 = \hat{q}, \quad \hat{Q}_2 = \hat{p}. \quad (3) \]
Inequality (1) takes the form
\[ \sum_{\alpha,\beta=1}^{2} c_\alpha^* c_\beta \langle \hat{Q}_\alpha \hat{Q}_\beta \rangle \geq 0; \quad \langle \hat{Q}_\alpha \hat{Q}_\beta \rangle = \text{Tr} \hat{\rho} \hat{Q}_\alpha \hat{Q}_\beta. \quad (4) \]
In view of the identity
\[ \langle \hat{Q}_\alpha \hat{Q}_\beta \rangle = \frac{1}{2} \langle \{\hat{Q}_\alpha, \hat{Q}_\beta\} \rangle + \frac{1}{2} \langle [\hat{Q}_\alpha, \hat{Q}_\beta] \rangle, \quad (5) \]
where we use, as usual, the symmetrized and commutator product, one can rewrite the positivity condition for quadratic form (4) in variables $c_\alpha$ as the positivity condition of the matrix of quadratic form, i.e.,
\[ \langle \hat{Q}_\alpha \hat{Q}_\beta \rangle \geq 0 \quad \text{or} \quad \left( \frac{1}{2} \langle \{\hat{Q}_\alpha, \hat{Q}_\beta\} \rangle + \frac{1}{2} \langle [\hat{Q}_\alpha, \hat{Q}_\beta] \rangle \right) \geq 0. \quad (6) \]
For the particular operator $\hat{F}$ given by (2), the above condition is the condition of positivity of the Hermitian matrix
\[ \left( \begin{array}{ll} \langle \hat{q}^2 \rangle & \frac{1}{2} \langle (\hat{q} \hat{p} + \hat{p} \hat{q}) \rangle - \frac{i}{2} \langle \hat{p}^2 \rangle \\ \frac{1}{2} \langle (\hat{q} \hat{p} + \hat{p} \hat{q}) \rangle + \frac{i}{2} \langle \hat{p}^2 \rangle & \langle \hat{p}^2 \rangle \end{array} \right) \geq 0. \quad (7) \]
In view of the Sylvester criterion for the positivity of the matrix, one has obvious inequalities
\[ \langle \hat{q}^2 \rangle \geq 0, \quad \langle \hat{p}^2 \rangle \geq 0 \]
and the uncertainty relation

\[ \langle q^2 \rangle \langle p^2 \rangle - \frac{1}{4} \langle (\hat{q}\hat{p} + \hat{p}\hat{q}) \rangle^2 \geq \frac{1}{4}, \quad \hbar = 1. \]  

(8)

Now if one replaces in (2) \( \hat{q} \rightarrow \hat{q} - \langle \hat{q} \rangle \), \( \hat{p} \rightarrow \hat{p} - \langle \hat{p} \rangle \), relation (8) is the Schrödinger–Robertson uncertainty relation

\[ \sigma_{qq} \sigma_{pp} - \sigma_{qp}^2 \geq \frac{1}{4}, \]

(9)

where the variances of position and momentum

\[ \sigma_{qq} = \langle q^2 \rangle - \langle q \rangle^2, \quad \sigma_{pp} = \langle p^2 \rangle - \langle p \rangle^2 \]  

(10)

and covariance of position and momentum

\[ \sigma_{qp} = \frac{1}{2} \langle (\hat{q}\hat{p} + \hat{p}\hat{q}) \rangle - \langle \hat{q} \rangle \langle \hat{p} \rangle \]  

(11)

are involved.

In the case of \( \langle \hat{q} \rangle = 0 \) and \( \langle \hat{p} \rangle = 0 \), inequalities (9) and (8) are equivalent.

For the multimode case, one takes the operator

\[ \hat{F} = \sum_{\alpha=1}^{2N} c_\alpha \hat{Q}_\alpha, \quad \hat{Q}_1 = \hat{q}_1, \hat{Q}_2 = \hat{q}_2, \ldots, \hat{Q}_N = \hat{q}_N, \hat{Q}_{N+1} = \hat{p}_1, \ldots, \hat{Q}_{2N} = \hat{p}_N. \]  

(12)

In this case, relation (11) provides the positivity condition for matrix (5) where \( \alpha, \beta = 1, \ldots, 2N \). This condition can be rewritten as the positivity of the matrix principal minors. The determinant of the matrix (last 2Nth principal minor) yields the weaker inequality

\[ \det \left( \frac{1}{2} \langle \hat{Q}_\alpha \hat{Q}_\beta + \hat{Q}_\beta \hat{Q}_\alpha \rangle \right) \geq \frac{1}{4^N}. \]  

(13)

### 3 Scaling transform as nonpositive map

There are completely positive and not completely positive linear maps of density operators [14]. Usually for detecting the entanglement one uses positive but not completely positive maps. In [10] we used the scaling transform to study the separability criterion for continuous variables.
Below we show that the scaling transform is a nonpositive transform. The scaling transform is defined through the transform of Wigner function

$$W(q, p) \rightarrow W_s(q, p) = |\lambda|^2 W(\lambda q, \lambda p). \quad (14)$$

The Wigner function is related to density matrix $\rho(x, x')$ in the position representation by the invertible map

$$W(q, p) = \int \rho \left( q + \frac{u}{2}, q - \frac{u}{2} \right) e^{-ipu} du \quad (15)$$

and

$$\rho(x, x') = \frac{1}{2\pi} \int W \left( \frac{x + x'}{2}, p \right) e^{ip(x-x')} dp. \quad (16)$$

For the case of $\text{Tr} \rho = 1$, one has the normalization condition

$$\int W(q, p) dq dp = 1. \quad (17)$$

One can see that if $W(q, p)$ satisfies the condition (17), due to the factor $|\lambda|^2$ in (14), we obtain

$$\int W_s(q, p) dq dp = 1. \quad (18)$$

One can use the squeezing transform

$$W(q, p) \rightarrow W^{sq}(q, p) = W(\kappa q, \kappa^{-1} p). \quad (19)$$

The squeezing transform is a unitary transform. Due to this, the nonnegative density operator is mapped by the squeezing transform onto another nonnegative density operator. The combination of transform (14) and squeezing transform provides the map of Wigner function used in [10]

$$W(q, p) \rightarrow W^{ps}(q, p) = |\lambda| W(q, \lambda p). \quad (20)$$

In fact, taking $\kappa^2 = \lambda^{-1}$ in (19) and making then transform (14) with scaling parameter $\sqrt{\lambda}$, we get (20).

Below we show that the transform (14) is also nonpositive. This means that (20) is also nonpositive since it is the product of nonpositive scaling transform and positive squeezing transform (14).

To show that the scaling transform is nonpositive, we calculate the fidelity

$$f = \text{Tr} \rho_0 \rho_1^{(s)} = \langle 0 | \rho_1^{(s)} | 0 \rangle, \quad (21)$$
where $\rho_0$ is density operator $|0\rangle\langle 0|$ of ground state $|0\rangle$ of harmonic oscillator and $\rho_1^{(s)}$ is the scaled density operator of the first excited state of the harmonic oscillator (we take $\hbar = m = \omega = 1$). The fidelity can be calculated in terms of overlap integral of Wigner functions of the corresponding states.

The Wigner function of the ground state reads (see, e.g., [6])

$$W_0(q, p) = 2e^{-q^2-p^2}. \quad (22)$$

The Wigner function of the first excited state reads

$$W_1(q, p) = 2(2q^2 + 2p^2 - 1)e^{-q^2-p^2}. \quad (23)$$

The scaled Wigner function depends on the parameter $\lambda$, i.e.,

$$W_1^{(s)}(q, p) = 2|\lambda|^2[2\lambda^2(q^2 + p^2) - 1]e^{-\lambda^2q^2-\lambda^2p^2}. \quad (24)$$

For small parameter $\lambda$, the leading term in (24) reads

$$W_1^{(s)}(q, p) \approx -2|\lambda|^2. \quad (25)$$

In view of this, the fidelity is

$$f = \int W_0(q, p)W_1^{(s)}(q, p) \frac{dq \, dp}{2\pi} \approx -2|\lambda|^2 < 0. \quad (26)$$

This means that at least one diagonal matrix element of scaled density operator is negative. Thus, for small parameters of scaling, the map under discussion is nonpositive.

Though we consider scaling map it is worth noting that there exists another map of density operators providing smoothed Wigner function from the initial one. For this map, one uses as convolution kernel some other Wigner function as it was shown in [15] this map is nonpositive for some choices of the Wigner function kernel. In particular, the convolution kernel based on Wigner function of the first excited state of the harmonic oscillator is of this kind.
4 Wigner–Weyl symbol of nonpositive Hermitian operator with fulfilling the uncertainty relation

In this section, we use the property of nonpositive map to present the Hermitian nonpositive operator $\hat{\rho}$ with $\text{Tr}\,\hat{\rho} = 1$ ($\hat{\rho} < 0$) fulfilling the condition

$$\begin{pmatrix}
\text{Tr}\,\hat{\rho}\hat{q}^2 & \text{Tr}\,\hat{\rho}_{1/2}^{1/2}(\hat{q}\hat{p} + \hat{p}\hat{q}) \\
\text{Tr}\,\hat{\rho}_{1/2}^{1/2}(\hat{q}\hat{p} + \hat{p}\hat{q}) & \text{Tr}\,\hat{\rho}\hat{p}^2
\end{pmatrix} > 0. \tag{27}
$$

In fact, this operator has matrix elements in the position representation determined by scaled Wigner function (24), i.e.,

$$\rho^{(s)}(x, x') = \frac{\lambda^2}{2\pi} \int \frac{2\lambda^2}{2} \left( \left( \frac{x + x'}{2} \right)^2 + p^2 \right) e^{-\lambda^2[(x+x')/2]^2 - \lambda^2p^2} e^{ip(x-x')} dp. \tag{28}
$$

This ”density” operator is negative but the variances and covariance of position and momentum read $(\langle q \rangle = 0, \langle p \rangle = 0)$

$$\begin{align*}
\sigma_{qq} &= \langle \hat{q}^2 \rangle = \frac{1}{\lambda^2}\sigma_{qq}^{(1)} = \frac{3}{2\lambda^2}, \\
\sigma_{qp} &= \frac{1}{2} (\hat{q}\hat{p} + \hat{p}\hat{q}) = 0, \tag{29} \\
\sigma_{pp} &= \langle \hat{p}^2 \rangle = \frac{1}{\lambda^2}\sigma_{pp}^{(1)} = \frac{3}{2\lambda^2}.
\end{align*}$$

Here $\sigma_{qq}^{(1)}$ and $\sigma_{pp}^{(1)}$ are quadrature dispersions in the first excited states of the harmonic oscillator.

The uncertainty relation is respected for $|\lambda| \leq 1$. Thus, for small scaling parameters, the uncertainty relation is fulfilled. Nevertheless, the ”density” operator used to calculate the dispersion matrix is nonpositive. Thus we demonstrated that fulfillment of the Schrödinger–Robertson uncertainty relation does not mean that the operator used as density operator must be positive. There can exist negative operators, for which matrix (7) calculated as if the operators $\hat{\rho}$ are density operators, is positive. Thus, the set of operators fulfilling the uncertainty relations in the form of positivity of matrix (7) is broader than the set of density states. To obtain the set of these operators, one needs to solve the inverse problem formulated as follows.
Given matrix (7). What are the operators which provide nonnegativity of this matrix?

The symplectic transform of positive density operators keeps the operators positive. The positivity of matrix (7) is invariant property with respect to symplectic transform. But there exist extra transforms belonging to general linear group which preserve the positivity of the matrix [16]. Scaling is just one of such transforms. Being expressed in terms of a map of density operators, these transforms provide the negative map respecting the uncertainty relations.

5 Separability criterion and nonpositive maps

The separable state of two-mode system is described by the density operator \( \hat{\rho}(1, 2) \) which can be represented as convex sum of simply separable states, i.e.,

\[
\hat{\rho}(1, 2) = \sum_k p_k \hat{\rho}^{(k)}(1) \otimes \hat{\rho}^{(k)}(2), \quad p_k \geq 0. \tag{30}
\]

The Wigner function of the separable state has the form

\[
W(q_1, p_1, q_2, p_2) = \sum_k p_k W^{(k)}(q_1, p_1) \tilde{W}^{(k)}(q_2, p_2). \tag{31}
\]

If one takes nonpositive partial scaling transform of the subsystem states

\[
\tilde{W}^{(k)}(q_2, p_2) \rightarrow |\lambda| \tilde{W}^{(k)}(q_2, \lambda p_2)
\]

suggested in [10], the uncertainty relation is respected for \(|\lambda| \leq 1\) which means that the initial nonnegative matrix

\[
\|A_{ij}\| = \begin{pmatrix}
\sigma_{q_1q_1} & \sigma_{q_1p_1} + \frac{i}{2} & \sigma_{q_1q_2} & \sigma_{q_1p_2} \\
\sigma_{p_1q_1} - \frac{i}{2} & \sigma_{p_1p_1} & \sigma_{p_1q_2} & \sigma_{p_1p_2} \\
\sigma_{q_2q_1} & \sigma_{q_2p_1} & \sigma_{q_2q_2} & \sigma_{q_2p_2} + \frac{i}{2} \\
\sigma_{p_2q_1} & \sigma_{p_2p_1} & \sigma_{p_2q_2} - \frac{i}{2} & \sigma_{p_2p_2}
\end{pmatrix} \geq 0 \tag{32}
\]

after the scaling transform takes the form

\[
\|A_{ij}^{(s)}\| = \begin{pmatrix}
\sigma_{q_1q_1} & \sigma_{q_1p_1} + \frac{i}{2} & \sigma_{q_1q_2} & \lambda^{-1}\sigma_{q_1q_2} \\
\sigma_{p_1q_1} - \frac{i}{2} & \sigma_{p_1p_1} & \sigma_{p_1q_2} & \lambda^{-1}\sigma_{p_1p_2} \\
\sigma_{q_2q_1} & \sigma_{q_2p_1} & \sigma_{q_2q_2} & \lambda^{-1}\sigma_{q_2p_2} + \frac{i}{2} \\
\lambda^{-1}\sigma_{p_2q_1} & \lambda^{-1}\sigma_{p_2p_1} & \lambda^{-1}\sigma_{p_2q_2} - \frac{i}{2} & \lambda^{-1}\sigma_{p_2p_2}
\end{pmatrix} \geq 0, \tag{33}
\]
and one must have for separable states

\[ \| A_{ij}^{(s)} \| \geq 0. \]  \hspace{1cm} (34)

Inequality (34) follows from the condition that each matrix

\[ \| A_{ij}^{(s)} \|^{(k)} \geq 0 \]  \hspace{1cm} (35)

and for separable states the convex sum of nonnegative matrices is nonnegative, i.e.,

\[ \| A_{ij}^{(s)} \| = \sum_k p_k \| A_{ij}^{(s)} \|^{(k)} \geq 0. \]  \hspace{1cm} (36)

In our consideration, we employ the condition \( \langle \hat{q} \rangle = 0, \langle \hat{p} \rangle = 0 \) but this condition can be removed. In fact, if in the initial state \( \langle \hat{q} \rangle \neq 0, \langle \hat{p} \rangle \neq 0 \), one can make local unitary shift transform which do not affect the entanglement properties. For new shifted density operators, one can apply the arguments presented above.

On the basis of experience to apply nonpositive scaling map for the detection of the entanglement, one can formulate general scheme of using negative maps to study the separability and entanglement.

To do this, one needs to generalize the procedure, in view of the uncertainty relation. In fact, if one has \( N^2 \) operators labeled as \( \hat{A}_{ij} \), \( j, k = 1, 2, \ldots, N \), one may construct the matrix

\[ \| A_{ij} \| = \| \text{Tr} (\hat{\rho} \hat{A}_{ij}) \|, \]  \hspace{1cm} (37)

where \( \hat{\rho} \) is any Hermitian operator (not necessarily a nonegative density operator). Having the set of operators \( \hat{\rho}_k \) one has the set of matrices

\[ \| A_{ij} \|^{(k)} = \| \text{Tr} (\hat{\rho}_k \hat{A}_{ij}) \|. \]  \hspace{1cm} (38)

Assume that \( \| A_{ij} \|^{(k)} \geq 0 \), then a convex combination is also nonnegative \( \sum_k p_k \| A_{ij} \|^{(k)} \geq 0 \). With the help of these remarks we return to the separability criterion.

Given separable state (30) of bipartite system, one can apply nonpositive \( \mathcal{N} \) map to the second-subsystem density matrix

\[ \hat{\rho}^{(k)}(2) \to \mathcal{N} \hat{\rho}^{(k)}(2) = \hat{\rho}_{\mathcal{N}}^{(k)}(2). \]  \hspace{1cm} (39)
This operation induces the map

\[ \hat{\rho}(1, 2) \rightarrow \hat{\rho}_N(1, 2). \]

The operator \( \hat{\rho}_N(2) \) can be nonpositive but we assume extra conditions, namely, there exist the set of operators \( \hat{A}_{ij} \) for which the numerical matrices

\[
\| \text{Tr} \hat{A}_{ij} \left( \hat{\rho}^{(k)}(1) \otimes \hat{\rho}^{(k)}(2) \right) \| \geq 0, \quad (40)
\]

\[
\| \text{Tr} \hat{A}_{ij} \left( \hat{\rho}^{(k)}(1) \otimes \hat{\rho}^{(k)}_N(2) \right) \| \geq 0. \quad (41)
\]

Then for separable states the convex sum of nonnegative matrices (41) yields

\[ \text{Tr} \| \hat{\rho}_N(1, 2) \hat{A}_{ij} \| \geq 0. \]

For entangled states, one can have violation of this inequality. Thus in our formulation of using nonpositive maps to detect the entanglement we introduce a new element. It is a set of operators \( \hat{A}_{ij} \) labeled by matrix indices. After tracing with some positive or negative operator \( \hat{\rho} \) the obtained numerical matrices must be positive. This means that we use the map \( \hat{\rho} \rightarrow \| A_{ij} \| \) of the Hermitian operators onto positive numerical matrices. This map can be realized in two steps. One step is the positive or nonpositive map \( \hat{\rho} \rightarrow \hat{\rho}_N \). The second step is \( \hat{\rho}_N \rightarrow \| A_{ij} \| = \text{Tr} \left( \hat{\rho}_N \hat{A}_{ij} \right). \)

Using such procedure one can extend the method of detecting the entanglement by means of positive but not completely positive maps to apply nonpositive maps to density operators of composed systems. Namely this ansatz is used for the partial scaling transform procedure.

6 Conclusions and Perspectives

To conclude, we formulate the main results of this study.

We have shown that fulfilling the Schrödinger–Robertson position–momentum uncertainty relation does not imply that the density operator is nonnegative, i.e., the uncertainty relation does not determine the quantum state. Fulfilling the uncertainty relation is necessary but not sufficient condition of nonnegativity of the density operator.

We presented the example of nonpositive operator (in the form of its Wigner–Weyl symbol) for which the uncertainty relation is fulfilled.
The obtained experience provided the possibility to formulate a procedure of detecting the entanglement of the multipartite system states using nonpositive maps of the subsystem density matrices.

It was emphasised that the partial scaling transform criterion suggested in [10] uses positive map of the position–momentum dispersion matrix induced by nonpositive map of density operator by means of scaling momentum in Wigner function.

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References


