Minimum-uncertainty states and completeness of non-negative quasiprobability of finite-dimensional quantum systems

T. Hashimoto, A. Hayashi, and M. Horibe
Department of Applied Physics, University of Fukui, Fukui 910-8507, Japan

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We construct minimum-uncertainty states and a non-negative quasiprobability distribution for quantum systems on a finite-dimensional space. We reexamine the theorem of Massar and Spindel for the uncertainty relation of the two unitary operators related by the discrete Fourier transformation. It is shown that some assumptions in their proof can be justified by the use of the Perron-Frobenius theorem. The minimum-uncertainty states are the ones that saturate this uncertainty inequality. The continuum limit is closely analyzed by introducing a scale factor in the limiting scheme. Using the minimum-uncertainty states, we construct a non-negative quasiprobability distribution. Its marginal distributions are smeared out. However, we show that this quasiprobability is optimal in the sense that there does not exist a non-negative quasiprobability distribution with sharper marginal properties if the translational covariance in the phase space is assumed. Generally, it is desirable that the quasiprobability is complete, i.e., it contains full information of the state. We show that the obtained quasiprobability is indeed complete if the dimension of the state space is odd, whereas it is not if the dimension is even.

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I. INTRODUCTION

The uncertainty principle [1] is arguably one of the most fundamental features that differentiate quantum mechanics from classical mechanics. It states that the product of uncertainties in complementary physical observables (e.g., position and momentum) has an inherent finite lower bound, and it has a profound influence on our view of the physical world. Because of the uncertainty principle, the dynamics of a quantum system is qualitatively different from a classical one; for example, an atom would collapse without this principle. Furthermore, recent studies show that the uncertainty principle also plays an important role in a variety of types of quantum information processings [2]. For example, quantum cryptography [3], one of the most remarkable applications of quantum information, exploits the uncertainty principle together with the no-cloning theorem [4] to ensure its provable security.

The uncertainty relation of the position and momentum in the continuous quantum mechanics is expressed by an inequality involving the standard deviations of their distributions [5]; that is, $\Delta x \Delta p \geqslant 1/2$. The states that attain the minimum are called minimum-uncertainty states, and they are given by the coherent states. The coherent states, the eigenstates of the annihilation operator, have interesting properties and useful applications in various fields of physics (see, e.g., Ref. [6]). Using the coherent states, one can define a quasiprobability distribution for the position and momentum variables, which is called the Husimi function (Q-distribution) [7]. The Husimi function is always non-negative, in contrast to the Wigner function [8], which is another quasidistribution function and may take negative values except for the case of Gaussian wave functions [9].

In this paper, we study analogous minimum-uncertainty states and a non-negative quasiprobability distribution for finite-dimensional quantum systems (qudits). To define the position and momentum coordinates, we take two bases related by the discrete Fourier transformation. The modulus of the expectation value of the position (momentum) translation operator is suitable for quantifying the uncertainty of the position (momentum) distribution [10–12]. For other approaches using the Jacobi θ function to construct analogous minimum-uncertainty states for a qudit, see, e.g., [13–15].

Massar and Spindel derived an inequality for the expectation values of the above two translation operators (Theorem 2 in [12]). They also discussed the minimum-uncertainty states saturating their inequality (Theorem 3 in [12]), which involves two assumptions for the greatest eigenvalue and the associated eigenvector of the Harper operator. We will show that these two assumptions can be justified using the Perron-Frobenius theorem (see, e.g., [16]), and we provide a detailed proof of a theorem combining those of Massar and Spindel (Sec. II B).

We call the states saturating this inequality minimum uncertainty states, which comprise an overcomplete set in the state space. In Sec. III, we will give a close analysis to show that these minimum-uncertainty states approach the coherent states as the dimension of the state space goes to infinity.

In the same way as in continuous quantum mechanics, we define a quasiprobability distribution of a qudit using the minimum-uncertainty states (Sec. IV). This is a finite-dimensional version of the Husimi function, and non-negative at the cost of the smeared-out marginal distributions. We show that the obtained quasiprobability distribution is optimal in the sense that there exists no non-negative quasiprobability distribution with sharper marginal properties if the translational covariance is assumed.

In continuous quantum mechanics the Husimi function is complete, i.e., it contains full information of the state. This is one of the desirable properties of quasiprobabilities of quantum systems. For finite-dimensional quantum systems, however, we find that the obtained quasiprobability is indeed complete if the dimension of the state space is odd, whereas it is not if the dimension is even (Sec. V).

II. MINIMUM-UNCERTAINTY STATES OF A FINITE-DIMENSIONAL QUANTUM SYSTEM

A. Position and momentum uncertainty of a qudit

We consider a qudit, a quantum system described by a d-dimensional complex linear space $\mathbb{C}^d$. An orthonormal basis $\{|a\rangle\}_{a=0}^{d-1}$ is fixed to define the "position" coordinate a. We introduce another orthonormal basis, which is the discrete Fourier transform defined by

$$|\tilde{b}\rangle = \frac{1}{\sqrt{d}} \sum_{a=0}^{d-1} \omega^{ba} |a\rangle , \; b = 0, 1, \ldots, \ldots, d-1, \quad (1)$$

where $\omega = e^{2\pi i/d}$ is a primitive dth root of unity. The index b is interpreted as the "momentum" coordinate. These two bases are unbiased in the sense that $|\langle a|\tilde{b}\rangle| = 1/\sqrt{d}$ for all a and b, and they are expected to approach the continuous position and momentum bases as the dimension d goes to infinity. As a feature of the discrete Fourier transform, the position and momentum coordinates, a and b, cannot simultaneously have sharp values.

To quantify the uncertainty with respect to these two bases, we employ two unitary operators Q and P. The operator Q is given by

$$Q = \sum_{a=0}^{d-1} \omega^{a} |a\rangle \langle a| , \quad (2)$$

which is diagonal in the position basis $\{|a\rangle\}$. In the momentum basis $\{|\tilde{b}\rangle\}$, the operator Q translationally shifts the momentum coordinate as $Q|\tilde{b}\rangle = |\widetilde{b+1}\rangle$. Here, it is assumed that if $b+1 = d$, then $|\widetilde{b+1}\rangle$ is equal to $|\tilde{0}\rangle$. Throughout this paper, we employ this periodic convention for the position and momentum coordinates; namely, we assume that

$$|a+d\rangle = |a\rangle , \; |\widetilde{b+d}\rangle = |\tilde{b}\rangle \quad (3)$$

for any integers a and b. Another operator P is defined by

$$P = \sum_{b=0}^{d-1} \omega^{-b} |\tilde{b}\rangle \langle \tilde{b}| , \quad (4)$$

which is diagonal in the momentum basis, and in the position basis it acts as the translational operator; $P|a\rangle = |a+1\rangle$. It is readily shown that P and Q satisfy the following relations:

$$Q^d = P^d = \mathbf{1}, \; QP = \omega PQ. \quad (5)$$

The relation $QP = \omega PQ$ can be regarded as the counterpart of the canonical commutation relation of the continuous position and momentum operators.

For a general state $|\phi\rangle$, we write

$$|\phi\rangle = \sum_{a=0}^{d-1} c_a |a\rangle = \sum_{b=0}^{d-1} \tilde{c}_b |\tilde{b}\rangle , \quad (6)$$

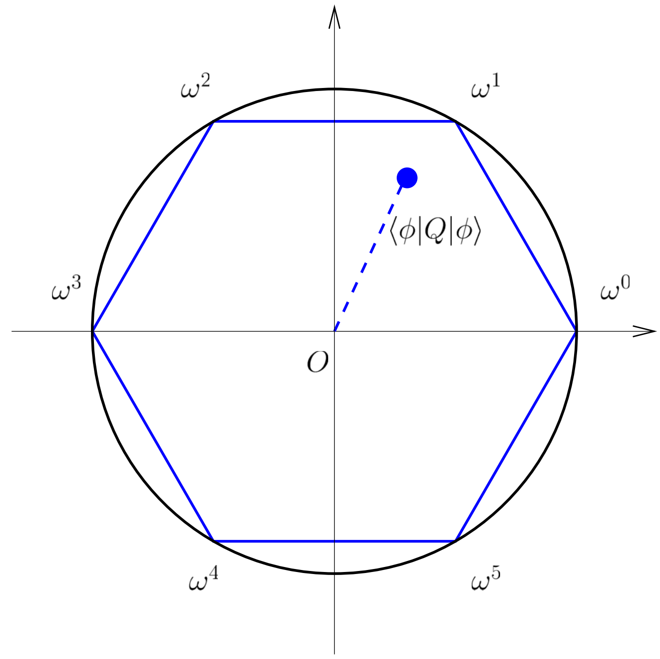

FIG. 1. The dth roots of unity in the complex plane and the expectation value $\langle\phi|Q|\phi\rangle$ represented by a point in the regular d-sided polygon formed by these roots. This figure displays the case of $d = 6$.

where c_a and $\tilde{c}_b$ are expansion coefficients in the position and momentum basis, respectively. Then the expectation values of Q and P for the state $|\phi\rangle$ take the following form:

$$\langle\phi|Q|\phi\rangle = \sum_{a=0}^{d-1} |c_a|^2 \omega^a = \sum_{b=0}^{d-1} \tilde{c}^*_{b+1} \tilde{c}_b, \quad (7)$$

$$\langle\phi|P|\phi\rangle = \sum_{a=0}^{d-1} c^*_{a+1} c_a = \sum_{b=0}^{d-1} |\tilde{c}_b|^2 \omega^{-b}. \quad (8)$$

Now let us examine the expectation value $\langle\phi|Q|\phi\rangle$ expressed in terms of c_a. This is an average of roots of unity ω^a with weights given by $|c_a|^2$. In the complex plane, the points $\{\omega^a\}_{a=0}^{d-1}$ are at the vertices of a regular d-sided polygon inscribed in the unit circle, and the expectation value $\langle\phi|Q|\phi\rangle$ is somewhere in this polygon (see Fig. 1). If the position coordinate has a sharp value, say a_0, $\langle\phi|Q|\phi\rangle$ is at the vertex ω^{a_0}. In this case, and only in this case, $|\langle\phi|Q|\phi\rangle|$ is equal to 1, otherwise we generally have $|\langle\phi|Q|\phi\rangle| < 1$. In contrast, if the weight is equally distributed as $|c_a|^2 = 1/d$, $\langle\phi|Q|\phi\rangle$ is at the origin; that is, $|\langle\phi|Q|\phi\rangle| = 0$. Thus the quantity $|\langle\phi|Q|\phi\rangle|$ is a measure of quantifying how sharply the position coordinate is distributed. In the same way, the quantity $|\langle\phi|P|\phi\rangle|$ measures the sharpness of the distribution of momentum coordinate. However, the quantities $|\langle\phi|Q|\phi\rangle|$ and $|\langle\phi|P|\phi\rangle|$ cannot simultaneously have their maximum value 1. For example, take the case of $|\langle\phi|Q|\phi\rangle| = 1$, which occurs only when $|c_a|$ is nonzero for a certain single value of a. In this case, however, $|\langle\phi|P|\phi\rangle|$ must be 0, as its expression in terms of c_a clearly shows.

Motivated by these considerations, we define the certainty C of a state $|\phi\rangle$ to be

$$C(|\phi\rangle) = |\langle\phi|Q|\phi\rangle\langle\phi|P|\phi\rangle| \tag{9}$$

to quantify the mutual uncertainty with respect to the position and momentum coordinates. Note that a larger C means less uncertainty as the name "certainty" indicates.

B. Minimum-uncertainty states

In the preceding section, we have seen that the certainty $C(|\phi\rangle)$ in Eq. (9) serves as a measure of certainty of position and momentum for a qudit state $|\phi\rangle$. In this section, we study the maximum value of the certainty and the states attaining the maximum certainty: the states with the minimum uncertainty.

Let us first examine the case of a qubit, $d = 2$. In the two-dimensional case, the operators Q and P are given by the Pauli matrices,

$$Q = |0\rangle\langle 0| - |1\rangle\langle 1| = \sigma_z,$$
$$P = |0\rangle\langle 1| + |1\rangle\langle 0| = \sigma_x.$$

The states are conveniently expressed by the Bloch vector representation,

$$|\boldsymbol{n}\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle, \tag{10}$$

where $\boldsymbol{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ is the Bloch vector. For the certainty C of the state $|\boldsymbol{n}\rangle$, we obtain

$$C(\boldsymbol{n}) = |\langle\boldsymbol{n}|\sigma_z|\boldsymbol{n}\rangle\langle\boldsymbol{n}|\sigma_x|\boldsymbol{n}\rangle| = |n_z n_x|. \tag{11}$$

The upper bound of $C(\boldsymbol{n})$ is readily determined by using the following inequalities:

$$|n_z n_x| \leqslant \frac{n_x^2 + n_z^2}{2} \leqslant \frac{1}{2}. \tag{12}$$

Thus the maximum value of the certainty C is $1/2$, and the maximum is attained by the following four Bloch vectors:

$$\boldsymbol{n}^{(\alpha,\beta)} = \frac{1}{\sqrt{2}}((-1)^\alpha, 0, (-1)^\beta)\ (\alpha,\beta = 0,1). \tag{13}$$

The state with $\boldsymbol{n}^{(0,0)}$ is denoted by $|\Gamma\rangle$, and it takes the following explicit form:

$$|\Gamma\rangle \equiv \cos\frac{\pi}{8}|0\rangle + \sin\frac{\pi}{8}|1\rangle$$
$$= \frac{\sqrt{2+\sqrt{2}}}{2}|0\rangle + \frac{\sqrt{2-\sqrt{2}}}{2}|1\rangle. \tag{14}$$

It should be noticed that the four states attaining the maximum C can be expressed as

$$|\alpha,\beta\rangle \equiv \sigma_x^\alpha\sigma_z^\beta|\Gamma\rangle\ (\alpha,\beta = 0,1). \tag{15}$$

Now we generalize these results to arbitrary-dimensional cases, and we establish the following theorem:

Theorem: For any normalized state $|\phi\rangle$:

(i) The certainty C is bounded by the inequality,

$$C(|\phi\rangle) \equiv |\langle\phi|Q|\phi\rangle\langle\phi|P|\phi\rangle| \leqslant h^2, \tag{16}$$

where h is the greatest eigenvalue of Harper operator H given by

$$H \equiv (P + P^\dagger + Q + Q^\dagger)/4. \tag{17}$$

(ii) Equality in (16) holds if and only if

$$|\phi\rangle = P^\alpha Q^\beta|\Gamma\rangle\ \text{(up to a global phase)}, \tag{18}$$

where $|\Gamma\rangle$ is the nondegenerate eigenstate of H with the greatest eigenvalue h, and α and β are integers ($\alpha,\beta = 0, 1, \dots, d-1$). The states $|\alpha,\beta\rangle \equiv P^\alpha Q^\beta|\Gamma\rangle$ are called the minimum-uncertainty states.

Statement (i) is essentially a special case ($\theta = \pi/4$) of Theorem 2 shown by Massar and Spindel in [12]. For later convenience, we give its proof below. Statement (ii) corresponds to theorem 3 in [12], which was proved by assuming that the greatest eigenvalue h of H is nondegenerate and the associated eigenstate satisfies $\langle a|\Gamma\rangle \neq 0$. We will show that these two assumptions can be justified using the Perron-Frobenius theorem, which will also be powerful when we later discuss the completeness of the quasiprobability. For an analysis of the eigenstructure of the Harper operator in terms of the crossing number, see [17].

1. Proof of statement (i) in the theorem

To prove statement (i) in the theorem, we start with an inequality,

$$\sqrt{|\langle\phi|Q|\phi\rangle\langle\phi|P|\phi\rangle|} \leqslant \tfrac{1}{2}(|\langle\phi|Q|\phi\rangle| + |\langle\phi|P|\phi\rangle|), \tag{19}$$

where the equality holds if and only if $|\langle\phi|Q|\phi\rangle| = |\langle\phi|P|\phi\rangle|$.

We write a given state $|\phi\rangle$ in the basis $\{|a\rangle\}$ as

$$|\phi\rangle = \sum_{a=0}^{d-1} c_a|a\rangle. \tag{20}$$

Replacing expansion coefficients c_a by their moduli $|c_a|$, we introduce a new state $|\phi'\rangle$ as

$$|\phi'\rangle = \sum_{a=0}^{d-1}|c_a||a\rangle = \sum_{b=0}^{d-1}\tilde{c}'_b|\tilde{b}\rangle, \tag{21}$$

where expansion coefficients of $|\phi'\rangle$ in the basis $\{|\tilde{b}\rangle\}$ are denoted by $\tilde{c}'_b$. We further define another state $|\phi''\rangle$ by replacing $\tilde{c}'_b$ by $|\tilde{c}'_b|$, that is,

$$|\phi''\rangle = \sum_{b=0}^{d-1}|\tilde{c}'_b||\tilde{b}\rangle. \tag{22}$$

Using Eqs. (7) and (8), we can readily show that the following relations hold:

$$\langle\phi'|P|\phi'\rangle \geqslant |\langle\phi|P|\phi\rangle|, \tag{23a}$$
$$\langle\phi'|Q|\phi'\rangle = \langle\phi|Q|\phi\rangle \tag{23b}$$

and

$$\langle\phi''|P|\phi''\rangle = \langle\phi'|P|\phi'\rangle, \tag{24a}$$
$$\langle\phi''|Q|\phi''\rangle \geqslant |\langle\phi'|Q|\phi'\rangle|. \tag{24b}$$

Note that $\langle\phi''|P|\phi''\rangle$ and $\langle\phi''|Q|\phi''\rangle$ are real, and therefore $\langle\phi''|P|\phi''\rangle = \langle\phi''|P^\dagger|\phi''\rangle$ and $\langle\phi''|Q|\phi''\rangle = \langle\phi''|Q^\dagger|\phi''\rangle$. Thus we have

$$\frac{|\langle\phi|Q|\phi\rangle| + |\langle\phi|P|\phi\rangle|}{2} \leqslant \langle\phi''|\,\frac{P+P^\dagger+Q+Q^\dagger}{4}\,|\phi''\rangle\,. \tag{25}$$

The right-hand side is clearly less than or equal to h, the greatest eigenvalue of H,

$$\langle\phi''|\,\frac{P+P^\dagger+Q+Q^\dagger}{4}\,|\phi''\rangle \leqslant h. \tag{26}$$

Combining this result and inequality (19), we obtain inequality (16).

2. Eigenstate of H with the greatest eigenvalue

Before proving statement (ii) of the theorem, we study the properties of the eigenstate of H with the greatest eigenvalue h. Some of them will be needed in the proof of statement (ii). We will show the following:

(a) The greatest eigenvalue h is positive and not degenerate. The phase of corresponding eigenstate $|\Gamma\rangle$ can be chosen such that $\langle a|\Gamma\rangle$ is real and strictly positive for all a.

(b) The eigenstate $|\Gamma\rangle$ is invariant under the Fourier transformation; $F|\Gamma\rangle = |\Gamma\rangle$, where F is the Fourier transform operator defined by

$$F = \sum_{a=0}^{d-1} |\tilde{a}\rangle\langle a|\,, \tag{27}$$

and hence $\langle a|\Gamma\rangle = \langle\tilde{a}|\Gamma\rangle = \langle -a|\Gamma\rangle$.

(c) The following relations hold:

$$\begin{aligned} h &= \langle\Gamma|Q|\Gamma\rangle = \langle\Gamma|Q^\dagger|\Gamma\rangle \\ &= \langle\Gamma|P|\Gamma\rangle = \langle\Gamma|P^\dagger|\Gamma\rangle\,. \end{aligned} \tag{28}$$

To show that the above statement (a) holds, some known properties of elementwise positive matrices will be employed. Here, we treat operators in the matrix representation based on the basis $\{|a\rangle\}_{a=0}^{d-1}$. We introduce a real symmetric matrix $H_\kappa \equiv H + \kappa\mathbf{1}$ with κ a real number. The off-diagonal part of H_κ is given by $(P+P^\dagger)/4$, all of whose elements are non-negative. The diagonal part, $(Q+Q^\dagger)/4 + \kappa\mathbf{1}$, is denoted D, and all of its diagonal elements are strictly positive for a sufficiently large κ. Now consider H_κ^{d-1} and expand it in terms of P, $P^\dagger$, and D. For any $i \leqslant j$, there is a term of the form $(P^\dagger/4)^{j-i} D^{d-1-j+i}$ that has a strictly positive (i, j) entry while other terms are elementwise non-negative. For the (j, i) entry, a similar argument can be applied. Thus the matrix H_κ^{d-1} is elementwise strictly positive.

Now recall that, according to the Perron-Frobenius theorem, the eigenvalue of the largest modulus of an elementwise strictly positive matrix is real and nondegenerate, and the associated eigenvector can be chosen to have strictly positive components (see, e.g., [16]). The eigenvalues of H_κ^{d-1} are clearly given by $(\kappa+\lambda_i)^{d-1}$, with λ_i being real eigenvalues of H. Thus we conclude that the greatest eigenvalue of H is not degenerate and the associated eigenstate $|\Gamma\rangle$ can be chosen so that $\langle a|\Gamma\rangle > 0$ for all a.

To show that $h > 0$, note that the trace of H is 0. In the case of $d > 1$, this is possible only when $h > 0$ since h is the unique greatest eigenvalue. When $d = 1$, it is evident that $h = 1$.

Now we show that $F|\Gamma\rangle = |\Gamma\rangle$. It is easy to show that $FQF^\dagger = P^\dagger$ and $FPF^\dagger = Q$, and hence H commutes with F. This implies that $|\Gamma\rangle$ is an eigenstate of F since the greatest eigenvalue h is not degenerate. The possible eigenvalues of F are 1, -1, i, and $-i$. This is because $F^2 = T$, where T is the reflection operator given by

$$T = \sum_{a=0}^{d-1} |-a\rangle\langle a|\,, \tag{29}$$

and T satisfies $T^2 = \mathbf{1}$. Assume that $F|\Gamma\rangle = f|\Gamma\rangle$ with f being 1, -1, i, or $-i$. This is explicitly written as

$$\sum_{a'=0}^{d-1} \langle a|F|a'\rangle\langle a'|\Gamma\rangle = f\langle a|\Gamma\rangle\,, \tag{30}$$

where $\langle a|F|a'\rangle = \omega^{aa'}/\sqrt{d}$. Setting $a = 0$, we observe

$$\frac{1}{\sqrt{d}}\sum_{a'=0}^{d-1}\langle a'|\Gamma\rangle = f\langle 0|\Gamma\rangle\,. \tag{31}$$

This requires that $f = 1$ since $\langle a|\Gamma\rangle > 0$ for all a. From $F|\Gamma\rangle = |\Gamma\rangle$, it immediately follows that $\langle a|\Gamma\rangle = \langle\tilde{a}|\Gamma\rangle = \langle -a|\Gamma\rangle$.

Further, the invariance $F|\Gamma\rangle = |\Gamma\rangle$ implies

$$\langle\Gamma|Q|\Gamma\rangle = \langle\Gamma|F^\dagger QF|\Gamma\rangle = \langle\Gamma|P|\Gamma\rangle\,. \tag{32}$$

Since $\langle a|\Gamma\rangle$ and $\langle\tilde{b}|\Gamma\rangle$ are real, $\langle\Gamma|P|\Gamma\rangle$ and $\langle\Gamma|Q|\Gamma\rangle$ are also real. We therefore find

$$\langle\Gamma|Q|\Gamma\rangle = \langle\Gamma|Q^\dagger|\Gamma\rangle = \langle\Gamma|P|\Gamma\rangle = \langle\Gamma|P^\dagger|\Gamma\rangle\,, \tag{33}$$

which shows that each one is equal to h. Thus we obtain Eq. (28).

Explicit analytical solutions of h and $|\Gamma\rangle$ in general dimensions have not been obtained, but some of the results in the low-dimensional cases are collected in [18].

3. Proof of statement (ii) in the theorem

"If part" is evident. When $|\phi\rangle = P^\alpha Q^\beta|\Gamma\rangle$, we find that

$$|\langle\phi|P|\phi\rangle| = |\langle\Gamma|P|\Gamma\rangle| = h, \tag{34}$$

$$|\langle\phi|Q|\phi\rangle| = |\langle\Gamma|Q|\Gamma\rangle| = h, \tag{35}$$

which shows that $|\phi\rangle$ satisfies the equality in (16).

Proving "only if part" is rather involved. Suppose that $|\phi\rangle$ satisfies the equality in (16). In the same way as in the proof of statement (i), we define $|\phi'\rangle$ and $|\phi''\rangle$ as follows:

$$|\phi\rangle = \sum_{a=0}^{d-1} c_a|a\rangle\,, \tag{36}$$

$$|\phi'\rangle = \sum_{a=0}^{d-1}|c_a|\,|a\rangle = \sum_{b=0}^{d-1}\tilde{c}'_b\,|\tilde{b}\rangle\,, \tag{37}$$

$$|\phi''\rangle = \sum_{b=0}^{d-1}|\tilde{c}'_b|\,|\tilde{b}\rangle\,. \tag{38}$$

This time the equality should hold in all inequalities in the proof of statement (i).

First we note that the equality in (26) is satisfied only if $|\phi''\rangle = |\Gamma\rangle$ up to a global phase since the greatest eigenvalue h is not degenerate.

Second we examine the equality in (24b), $\langle\phi''|Q|\phi''\rangle = |\langle\phi'|Q|\phi'\rangle|$. This is explicitly written as

$$\sum_{b=0}^{d-1}|\tilde{c}'_{b+1}||\tilde{c}'_b| = \left|\sum_{b=0}^{d-1}\tilde{c}'^{*}_{b+1}\tilde{c}'_b\right|, \tag{39}$$

which implies that all terms on the right-hand side must have the same phase factor, that is, $\tilde{c}'^{*}_{b+1}\tilde{c}'_b = |\tilde{c}'_{b+1}\tilde{c}'_b|u$, with u being a complex number of unit modulus. This relation can be rewritten as

$$\frac{\tilde{c}'_b}{|\tilde{c}'_b|} = u\frac{\tilde{c}'_{b+1}}{|\tilde{c}'_{b+1}|}\ (b = 0, 1, \ldots, d-1). \tag{40}$$

Note that $|\tilde{c}'_b| > 0$ for all b since $|\phi''\rangle = |\Gamma\rangle$, and the above relation is well-defined. Using this relation successively, we obtain

$$\frac{\tilde{c}'_b}{|\tilde{c}'_b|} = u^{-b}\frac{\tilde{c}'_0}{|\tilde{c}'_0|}. \tag{41}$$

Setting $b = d$ and remembering $\tilde{c}'_d = \tilde{c}'_0$ by our convention, we find that the phase factor u must be a dth root of unity, ω^{α} with some integer α. Thus the b dependence of the phase of $\tilde{c}'_b$ is given by $\omega^{-\alpha b}$, from which we conclude that $|\phi'\rangle = P^{\alpha}|\phi''\rangle = P^{\alpha}|\Gamma\rangle$ up to a global phase.

Let us now turn to the equality in (23a), $\langle\phi'|P|\phi'\rangle = |\langle\phi|P|\phi\rangle|$, which is explicitly written as

$$\sum_{a=0}^{d-1}|c_{a+1}||c_a| = \left|\sum_{a=0}^{d-1}c^{*}_{a+1}c_a\right|. \tag{42}$$

Since $|\phi'\rangle = P^{\alpha}|\Gamma\rangle$, we have $|c_a| > 0$ for all a. We can repeat a similar argument to the preceding one, and we find that $|\phi\rangle$ is given by $Q^{\beta}|\phi'\rangle$ with some integer β. Combining this and the previous result, $|\phi'\rangle = P^{\alpha}|\Gamma\rangle$, we finally conclude that $|\phi\rangle = P^{\alpha}Q^{\beta}|\Gamma\rangle$ up to a global phase.

It should be noted that we used the fact that $\langle a|\Gamma\rangle \neq 0$ and $\langle\tilde{b}|\Gamma\rangle \neq 0$ for all a and b in the above argumentation.

4. Parameter θ in the theorem of Massar and Spindel

Theorems 2 and 3 in [12] involve a parameter $\theta \in [0, \pi/2]$. They state that for any $|\phi\rangle$ the following inequality holds:

$$\cos\theta|\langle\phi|Q|\phi\rangle| + \sin\theta|\langle\phi|P|\phi\rangle| \leqslant h_\theta, \tag{43}$$

where h_θ is the greatest eigenvalue of the Hermitian operator

$$H_\theta = \cos\theta\frac{P+P^\dagger}{2} + \sin\theta\frac{Q+Q^\dagger}{2}, \tag{44}$$

and the equality in Eq. (43) holds if and only if

$$|\phi\rangle = P^{\alpha}Q^{\beta}|\Gamma_\theta\rangle\ \text{(up to a global phase)}, \tag{45}$$

where $|\Gamma_\theta\rangle$ is the nondegenerate eigenstate of H_θ with the eigenvalue h_θ. In this paper, we have concentrated on the case $\theta = \pi/4$. It is, however, clear that the two assumptions in the proof of "only if part" can be justified as in the case $\theta = \pi/4$. This is because, except for the trivial cases $\theta = 0$ or $\theta = \pi/2$, the matrix $(H_\theta + \kappa\mathbf{1})^{d-1}$ can be shown elementwise to be strictly positive, and therefore h_θ is nondegenerate, $\langle a|\Gamma_\theta\rangle \neq 0$, and $\langle\tilde{b}|\Gamma_\theta\rangle \neq 0$.

III. CONTINUUM LIMIT

In the continuous quantum mechanics, the minimum-uncertainty states are given by coherent states, which are eigenstates of the annihilation operator, and by translationally shifting the ground state of a harmonic oscillator in the phase space. The minimum-uncertainty state $|\Gamma\rangle$ is expected to approach a coherent state as the dimension d goes to infinity (see, e.g., [12,17]). The coherent states, however, may have any width, and they are all minimum-uncertainty states in continuous quantum mechanics. In this section, introducing a scale factor in the limiting scheme, we show how the single state $|\Gamma\rangle$ approaches coherent states with different widths.

We start by writing the eigenequation $H|\phi\rangle = \lambda|\phi\rangle$ in the position basis $\{|a\rangle\}$,

$$\frac{1}{4}\left[c_{a+1} + c_{a-1} + 2\cos\left(\frac{2\pi}{d}a\right)c_a\right] = \lambda c_a, \tag{46}$$

where $c_a = \langle a|\phi\rangle$. Dickinson and Steiglitz [19] realized that Eq. (46) is a discrete version of the Mathieu equation by identifying $c_{a+1} - 2c_a + c_{a-1}$ with the central second difference. To extend this idea further, we consider the following limit: By introducing the lattice constant ϵ, we define the system size $L = \epsilon d$. The system size L and the dimension d go to infinity, and the lattice constant ϵ goes to zero, while $\sigma \equiv \sqrt{\epsilon L/(2\pi)}$ is fixed. It is this σ that determines the scale of length. The factor 2π in the definition of σ is just for later convenience. The position variable x is defined by $x = a\epsilon$. Here the range of the discrete position index a is taken to be $\lfloor -(d-1)/2\rfloor \leqslant a \leqslant \lfloor (d-1)/2\rfloor$, where the symbol $\lfloor\cdot\rfloor$ means the floor function. This ensures that, in the large-d limit, x becomes a continuous variable ranging from $-\infty$ to $+\infty$. Note that in this scheme we have

$$O(\epsilon^2) = O(1/L^2) = O(1/d). \tag{47}$$

Now we rewrite Eq. (46) as

$$-\frac{1}{2}\frac{\delta^2 c_a}{\epsilon^2} + \frac{2}{\epsilon^2}\sin^2\left(\frac{\pi}{d}a\right)c_a = \frac{2}{\epsilon^2}(1-\lambda)c_a, \tag{48}$$

where δ^2 is the central second difference given by

$$\delta^2 c_a = c_{a+1} - 2c_a + c_{a-1}. \tag{49}$$

By introducing the wave function $\phi(x) = c_a\sqrt{\epsilon}$, we observe

$$\frac{\delta^2 c_a}{\epsilon^2}\sqrt{\epsilon} = \phi''(x) + O\left(\frac{1}{d}\right) \tag{50}$$

and

$$\frac{2}{\epsilon^2}\sin^2\left(\frac{\pi}{d}a\right) = \frac{x^2}{2\sigma^4} + O\left(\frac{1}{d}\right). \tag{51}$$

Thus, in the leading order, Eq. (48) takes the form

$$-\frac{1}{2}\phi''(x) + \frac{x^2}{2\sigma^4}\phi(x) = \frac{2}{\epsilon^2}(1-\lambda)\phi(x), \tag{52}$$

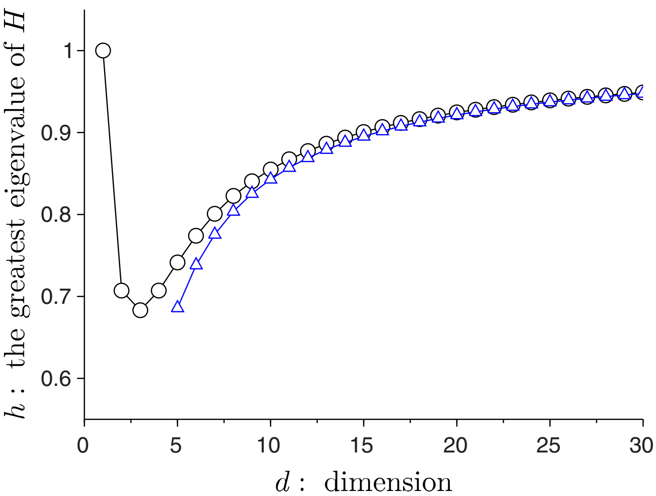

FIG. 2. The greatest eigenvalue h of the operator H vs dimension d. The circles represent the exact values calculated by diagonalizing H analytically or numerically. The values of the asymptotic formula Eq. (54) are plotted by triangles.

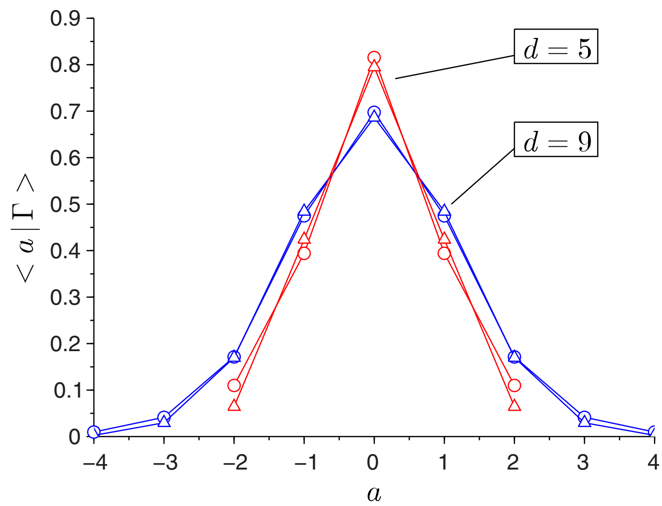

FIG. 3. The components of the minimum-uncertainty state $|\Gamma\rangle$. The components in the position basis $\{|a\rangle\,,\ -(d-1)/2 \leqslant a \leqslant (d-1)/2\}$ are plotted vs a for the $d=5$ and 9 cases. The circles are the values obtained by numerical calculations. The triangles represent the values by the asymptotic form of Eq. (56). The normalization constants $\mathcal{N}$ are determined numerically.

which is the Schrödinger equation of the harmonic oscillator with the angular frequency given by $1/\sigma^2$. The eigenenergy of this harmonic oscillator is given by $(n+1/2)/\sigma^2$, where $n = 0, 1, \ldots$. We thus find

$$\lambda = 1 - \left(n + \frac{1}{2}\right)\frac{\pi}{d}, \tag{53}$$

from which we obtain the asymptotic expression of the greatest eigenvalue h to be

$$h = 1 - \frac{\pi}{2d} \quad (\text{as } d \to \infty). \tag{54}$$

The corresponding ground-state wave function is given by a Gaussian function

$$\phi(x) \propto \exp\left(-\frac{x^2}{2\sigma^2}\right) = \exp\left(-\frac{\pi}{d}a^2\right). \tag{55}$$

Thus the asymptotic form of the minimum-uncertainty state $|\Gamma\rangle$ is given by

$$\langle a|\Gamma\rangle = \mathcal{N} \exp\left(-\frac{\pi}{d}a^2\right) \ (\text{as } d \to \infty), \tag{56}$$

where $[-(d-1)/2] \leqslant a \leqslant [(d-1)/2]$, and $\mathcal{N}$ is a normalization constant.

In Fig. 2, we compare the exact values of h with those obtained by the asymptotic formula Eq. (54). This shows that the asymptotic form is already a rather good approximation for relatively low dimensions. The components of the minimum-uncertainty state $\langle a|\Gamma\rangle$, the values by numerical calculation and by the asymptotic form Eq. (56), are plotted in Fig. 3. We see that the asymptotic form provides an unexpectedly good approximation even for the $d = 5$ case.

We briefly sketch how the inequality (16) of the certainty $C(\phi)$ is reduced to the usual uncertainty relation of the position and momentum variables in the continuum limit. First we analyze the expectation value $\langle\phi|Q|\phi\rangle$. In the continuum limit, the summation over a becomes an integral over x, and the exponential function $\exp(i\frac{2\pi}{d}a) = \exp(i\frac{2\pi}{L}x)$ can be expanded. Thus we have

$$\begin{aligned}\langle\phi|Q|\phi\rangle &= \sum_a e^{i\frac{2\pi}{d}a}|c_a|^2 \\ &= 1 + i\frac{2\pi}{L}\langle\hat{x}\rangle - \frac{1}{2}\left(\frac{2\pi}{L}\right)^2\langle\hat{x}^2\rangle + O\left(\frac{1}{d^{3/2}}\right),\end{aligned} \tag{57}$$

where

$$\langle\hat{x}\rangle = \int dx\, \phi^*(x)x\phi(x),$$

$$\langle\hat{x}^2\rangle = \int dx\, \phi^*(x)x^2\phi(x).$$

The modulus of $\langle\phi|Q|\phi\rangle$ then takes the form

$$|\langle\phi|Q|\phi\rangle| = 1 - \frac{\pi}{\sigma^2 d}(\Delta x)^2 + O\left(\frac{1}{d^{3/2}}\right), \tag{58}$$

in terms of the standard deviation of position coordinate defined by $\Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2}$. Similarly, $|\langle\phi|P|\phi\rangle|$ is expressed as

$$|\langle\phi|P|\phi\rangle| = 1 - \frac{\pi\sigma^2}{d}(\Delta p)^2 + O\left(\frac{1}{d^{3/2}}\right), \tag{59}$$

where Δp is the usual standard deviation of momentum coordinate. Meanwhile, the asymptotic form of h has already been obtained in Eq. (54). Combining all these results, we find that the inequality (16) of the certainty $C(\phi)$ is reduced to

$$\frac{1}{\sigma^2}(\Delta x)^2 + \sigma^2(\Delta p)^2 \geqslant 1 \tag{60}$$

in the leading order of $1/d$.

It is evident that, for a given wave function $\phi(x)$, the scale factor σ is arbitrary, since σ is a sort of artifact in the procedure of the continuum-limit scheme. The left-hand side of the above inequality (60) takes the minimum value $2\Delta x\Delta p$ when $\sigma = \sqrt{\Delta x/\Delta p}$. Thus we arrive at the usual uncertainty relation of the position and momentum variables,

$$\Delta x\Delta p \geqslant \tfrac{1}{2}. \tag{61}$$

IV. NON-NEGATIVE QUASIPROBABILITY AND ITS OPTIMALITY

The minimum-uncertainty states are defined as

$$|\alpha,\beta\rangle = P^\alpha Q^\beta |\Gamma\rangle \quad (\alpha,\beta = 0,1,\ldots,d-1). \tag{62}$$

The position and momentum distributions of $|\alpha,\beta\rangle$ are given by

$$|\langle a|\alpha,\beta\rangle|^2 = \Gamma_{a-\alpha}^2, \tag{63}$$

$$|\langle\tilde{b}|\alpha,\beta\rangle|^2 = \Gamma_{b-\beta}^2. \tag{64}$$

Note that $\Gamma_a \equiv \langle a|\Gamma\rangle$ has a peak at $a=0$, which can be seen from the analytical results in the low-dimensional cases and the numerical results for higher dimensions. Therefore, the position and momentum distribution of $|\alpha,\beta\rangle$ have a peak at $a=\alpha$ and $b=\beta$, respectively.

The d^2 minimum-uncertainty states $|\alpha,\beta\rangle$ are not mutually orthogonal, but they comprise an overcomplete set in the state vector space $\mathbb{C}^d$. The completeness relation of $|\alpha,\beta\rangle$ takes the form

$$\frac{1}{d}\sum_{\alpha,\beta=0}^{d-1} |\alpha,\beta\rangle\langle\alpha,\beta| = \mathbf{1}. \tag{65}$$

To derive this completeness relation, we employ the following useful identity, which holds for any operator Ω:

$$\sum_{\alpha,\beta=0}^{d-1} \omega^{\alpha b-\beta a} P^\alpha Q^\beta \Omega Q^{-\beta} P^{-\alpha} = d\,\mathrm{tr}[Q^{-b}P^{-a}\Omega]P^a Q^b, \tag{66}$$

or equivalently,

$$P^\alpha Q^\beta \Omega Q^{-\beta}P^{-\alpha} = \frac{1}{d}\sum_{a,b=0}^{d-1} \omega^{-\alpha b+\beta a}\mathrm{tr}[Q^{-b}P^{-a}\Omega]P^a Q^b. \tag{67}$$

This identity can be obtained by using the commutation relation $QP=\omega PQ$ together with the mutual orthogonality and completeness of the set of operators $\{P^\alpha Q^\beta\}_{\alpha,\beta=0}^{d-1}$ in the operator space. Setting $a=b=0$ and $\Omega = |\Gamma\rangle\langle\Gamma|$ in the above identity (66), we obtain the completeness of the minimum-uncertainty states (65).

Based on these observations, it is reasonable to define the quasiprobability distribution $D(\alpha,\beta)$ for a given state ρ with respect to the position and momentum coordinates α and β as follows:

$$D(\alpha,\beta) \equiv \frac{1}{d}\langle\alpha,\beta|\rho|\alpha,\beta\rangle = \mathrm{tr}[\rho\Delta(\alpha,\beta)], \tag{68}$$

where we introduced the phase point operator $\Delta(\alpha,\beta)$ given by

$$\Delta(\alpha,\beta) = \frac{1}{d}|\alpha,\beta\rangle\langle\alpha,\beta|. \tag{69}$$

Note that $D(\alpha,\beta)$ is non-negative and normalized to unity when summed over all phase-space points (α,β). However, the states $|\alpha,\beta\rangle$ are not mutually orthogonal, and therefore distinct phase-space points (α,β) are not regarded as exclusive events. This is the reason why we call $D(\alpha,\beta)$ a *quasi*probability distribution.

The phase point operator $\Delta(\alpha,\beta)$ satisfies the following relations if summed over α or β:

$$\sum_{\beta=0}^{d-1}\Delta(\alpha,\beta) = \sum_{a=0}^{d-1}\Gamma_{a-\alpha}^2|a\rangle\langle a|, \tag{70}$$

$$\sum_{\alpha=0}^{d-1}\Delta(\alpha,\beta) = \sum_{b=0}^{d-1}\Gamma_{b-\beta}^2|\tilde{b}\rangle\langle\tilde{b}|. \tag{71}$$

The first equation (70) can be obtained by summing over β in Eq. (67) with $\Omega = |\Gamma\rangle\langle\Gamma|$. Similarly, the second equation (71) also follows from Eq. (67). These relations (70) and (71) imply that the quasiprobability distribution $D(\alpha,\beta)$ has the following marginal distributions:

$$\sum_{\beta=0}^{d-1}D(\alpha,\beta) = \sum_{a=0}^{d-1}\Gamma_{a-\alpha}^2\langle a|\rho|a\rangle, \tag{72}$$

$$\sum_{\alpha=0}^{d-1}D(\alpha,\beta) = \sum_{b=0}^{d-1}\Gamma_{b-\beta}^2\langle\tilde{b}|\rho|\tilde{b}\rangle. \tag{73}$$

We find that the marginal distributions are smeared out in the sense that $D(\alpha,\beta)$ summed over β, for example, gives the weighted average of $\langle a|\rho|a\rangle$ with the weight centered at $a=\alpha$.

It is evident that the phase point operator $\Delta(\alpha,\beta)$ respects the translational covariance,

$$P^a Q^b \Delta(\alpha,\beta)Q^{-b}P^{-a} = \Delta(\alpha+a,\beta+b), \tag{74}$$

which implies that if $D(\alpha,\beta)$ are the quasiprobabilities of a state ρ, then the quasiprobabilities of $\rho' = P^aQ^b\rho Q^{-b}P^{-a}$ are given by $D(\alpha-a,\beta-b)$. The phase point operator is also covariant under the Fourier transformation, i.e., $F\Delta(\alpha,\beta)F^\dagger = \Delta(-\beta,\alpha)$, but not covariant under the more general symplectic transformation considered in [20–22].

For the odd-dimensional system, the Wigner function of Wootters [23] and Cohendet *et al.* [24] is defined as $D_W(\alpha,\beta) = \mathrm{tr}[\rho\Delta_W(\alpha,\beta)]$ with the phase point operator given by

$$\Delta_\mathrm{W}(\alpha,\beta) = \frac{1}{d}P^\alpha Q^\beta T Q^{-\beta}P^{-\alpha}. \tag{75}$$

This Wigner function has sharp marginal distributions since

$$\sum_{\beta=0}^{d-1}\Delta_W(\alpha,\beta) = |\alpha\rangle\langle\alpha|, \tag{76}$$

$$\sum_{\alpha=0}^{d-1}\Delta_W(\alpha,\beta) = |\tilde{\beta}\rangle\langle\tilde{\beta}|. \tag{77}$$

However, the Wigner functions $D_W(\alpha,\beta)$ may take negative values, and they are non-negative only for special states called stabilizer states [21], since $\Delta_W(\alpha,\beta)$ is not positive-semidefinite. Using the mutual orthogonality and completeness of $\Delta_W(\alpha, \beta)$ in the operator space, we can easily express $\Delta(\alpha, \beta)$ in terms of $\Delta_W(\alpha, \beta)$. The result is given by

$$\Delta(\alpha, \beta) = \sum_{\alpha', \beta'=0}^{d-1} w(\alpha - \alpha', \beta - \beta')\Delta_W(\alpha', \beta'), \tag{78}$$

where

$$w(\alpha, \beta) = \langle\Gamma|\Delta_W(\alpha, \beta)|\Gamma\rangle . \tag{79}$$

We see that the phase point operator $\Delta(\alpha, \beta)$ built with the minimum-uncertainty states can be written in the form of convolution of the weight $w(\alpha, \beta)$ and $\Delta_W(\alpha, \beta)$, and thus it acquires non-negativity at the cost of losing the sharp marginal property.

The quasiprobability distribution based on the minimum-uncertainty states is non-negative, but its marginal distributions are smeared out, as shown in Eqs. (72) and (73). A natural question is whether there exists a non-negative quasiprobability distribution that satisfies sharper marginal conditions. In what follows, we show that the answer is "no" as long as the translational covariance in the phase space is assumed.

Let $\Lambda(\alpha, \beta)$ be phase point operators of a non-negative quasiprobability distribution with the translational covariance. To quantify the sharpness of the marginal distributions, we define

$$\sigma \equiv \left|\mathrm{tr}\left[\sum_{\beta=0}^{d-1} \Lambda(\alpha, \beta)Q\right]\right|, \tag{80}$$

$$\tau \equiv \left|\mathrm{tr}\left[\sum_{\alpha=0}^{d-1} \Lambda(\alpha, \beta)P\right]\right|. \tag{81}$$

Because of the translational covariance, σ and τ are independent of α and β, respectively. In the case of $\Delta_W(\alpha, \beta)$ by Wootters and Cohendet *et al.*, we find that $\sigma = \tau = 1$ since the marginal conditions are perfectly sharp, as shown in Eqs. (76) and (77). However, for $\Delta(\alpha, \beta)$ based on the minimum-uncertainty states, we have $\sigma = \tau = h$, which is less than 1 if $d \geqslant 2$.

The translational covariance implies that $\Lambda(\alpha, \beta)$ can be written as

$$\Lambda(\alpha, \beta) = \frac{1}{d} P^\alpha Q^\beta K Q^{-\beta} P^{-\alpha}, \tag{82}$$

where $K = d\Lambda(0, 0)$ is a Hermitian operator with $\mathrm{tr}\, K = 1$ since $\Lambda(\alpha, \beta)$ should be Hermitian and normalized as $\sum_{\alpha,\beta=0}^{d-1} \Lambda(\alpha, \beta) = 1$. In addition, K should be positive-semidefinite to ensure that the quasiprobabilities are non-negative. Thus K can be regarded as a state on $\mathbb{C}^d$. In terms of K, the measures of sharpness, σ and τ, take the following simple form:

$$\sigma = |\mathrm{tr}[KQ]|, \ \tau = |\mathrm{tr}[KP]|. \tag{83}$$

Here it should be noticed that the theorem in Sec. II B holds also for mixed states; that is, for any state ρ, we have

$$|\mathrm{tr}[\rho Q]\mathrm{tr}[\rho P]| \leqslant h^2, \tag{84}$$

where the equality holds if and only if $\rho = |\alpha, \beta\rangle\langle\alpha, \beta|$. This can be shown by the following inequalities:

$$\begin{aligned} |\mathrm{tr}[\rho Q]\mathrm{tr}[\rho P]|^{1/2} &\leqslant \frac{1}{2}(|\mathrm{tr}[\rho Q]| + |\mathrm{tr}[\rho P]|) \\ &\leqslant \sum_i r_i \frac{1}{2}(|\langle\phi_i|Q|\phi_i\rangle| + |\langle\phi_i|P|\phi_i\rangle|) \leqslant h, \end{aligned} \tag{85}$$

where we used the spectral decomposition $\rho = \sum_i r_i |\phi_i\rangle\langle\phi_i|$.

Using this extended theorem, we obtain

$$\sigma\tau \leqslant h^2, \tag{86}$$

where the equality holds if and only if $K = |\alpha_0, \beta_0\rangle\langle\alpha_0, \beta_0|$ with $\alpha_0, \beta_0 = 0, 1, \ldots, d-1$. This implies that the upper bound of the sharpness $\sigma\tau$ is attained by $\Lambda(\alpha, \beta) = \Delta(\alpha + \alpha_0, \beta + \beta_0)$. Thus we conclude that the quasiprobability distribution based on $\Delta(\alpha, \beta)$ is optimal and unique up to a cyclic relabeling of the position and momentum coordinates; $\alpha \to \alpha + \alpha_0$ and $\beta \to \beta + \beta_0$.

V. COMPLETENESS

It is desirable that the quasiprobability distribution completely determines the state of the system. This requires that the set of phase point operators $\{\Delta(\alpha, \beta)\}_{\alpha,\beta=0}^{d-1}$ should be complete in the operator space. To see this, we calculate the Fourier transform of $\Delta(\alpha, \beta)$,

$$\begin{aligned} \tilde{\Delta}(m, n) &\equiv \frac{1}{d}\sum_{\alpha,\beta=0}^{d-1} \omega^{\alpha n - \beta m}\Delta(\alpha, \beta) \\ &= \frac{1}{d}\langle\Gamma|Q^{-n}P^{-m}|\Gamma\rangle P^m Q^n \\ &= \frac{1}{d}\langle\Gamma|Q^n P^m|\Gamma\rangle P^m Q^n. \end{aligned} \tag{87}$$

We employed Eq. (66) with $\Omega = |\Gamma\rangle\langle\Gamma|$ to obtain the second line of the above equation, and the reflection symmetry $T|\Gamma\rangle = |\Gamma\rangle$ was also used in the last line. Since the set of operators $\{P^m Q^n\}_{m,n=0}^{d-1}$ is complete, the completeness of the phase point operators is equivalent to the conditions given by

$$f_{m,n} \equiv \langle\Gamma|P^m Q^n|\Gamma\rangle \neq 0 \ (m, n = 0, 1, \ldots, d-1). \tag{88}$$

f_{mn} has the following symmetries:

$$\begin{aligned} f_{mn} &= f_{-m,-n}, \\ f_{mn} &= f_{nm}, \\ f_{mn} &= \omega^{-mn} f_{m,-n}, \\ f_{mn} &= \omega^{-mn} f^*_{mn}. \end{aligned}$$

We used the fact that the state $|\Gamma\rangle$ is invariant under the Fourier transformation, and components $\langle a|\Gamma\rangle$ can be taken to be real values.

Here we have different results depending on whether the dimension d is even or odd. When d is even, some of the conditions (88) are clearly violated. For example, we find that

$$\langle\Gamma|P^{d/2}Q^{d/2}|\Gamma\rangle = \frac{1}{2h}\langle\Gamma|\{P^{d/2}Q^{d/2}, H\}|\Gamma\rangle = 0, \tag{89}$$

since the operator $P^{d/2}Q^{d/2}$ anticommutes with H. Using the symmetries of f_{mn}, we also observe that

$$\langle\Gamma|P^m Q^{d/2}|\Gamma\rangle = 0\ (m = \text{odd}), \tag{90a}$$

$$\langle\Gamma|P^{d/2} Q^n|\Gamma\rangle = 0\ (n = \text{odd}). \tag{90b}$$

We remark that it is only in those cases that $\langle\Gamma|P^m Q^n|\Gamma\rangle$ vanishes, which can be shown by an analysis similar to the one in the odd-dimensional case given later in this section. Thus, the phase point operators $\Delta(\alpha,\beta)$ are not complete if d is even. Let us examine the qubit ($d = 2$) case more closely. In this case, we can write the phase point operator as

$$\Delta(\alpha,\beta) = \tfrac{1}{4}(1 + \boldsymbol{n}^{(\alpha,\beta)}\cdot\boldsymbol{\sigma})\ (\alpha,\beta = 0,1), \tag{91}$$

where the Bloch vectors $\boldsymbol{n}^{(\alpha,\beta)}$ are given in Eq. (13). Since the y-components of $\boldsymbol{n}^{(\alpha,\beta)}$ are 0, the set of $\Delta(\alpha,\beta)$'s is not complete in the whole qubit space. However, it is interesting that it is still complete in the qubit space of real amplitudes.

When d is odd, on the other hand, the conditions (88) are satisfied: the set of phase point operators $\Delta(\alpha,\beta)$ is complete, which will be shown in the rest of this section.

A. Equations for $\langle\Gamma|P^m Q^n|\Gamma\rangle$

In this subsection, we will derive some equations fulfilled by $f_{mn} \equiv \langle\Gamma|P^m Q^n|\Gamma\rangle$. Here, the dimension d is arbitrary (odd or even).

We begin with the following two evident equations:

$$\langle\Gamma|HP^m Q^n|\Gamma\rangle = h\,\langle\Gamma|P^m Q^n|\Gamma\rangle, \tag{92a}$$

$$\langle\Gamma|P^m Q^n H|\Gamma\rangle = h\,\langle\Gamma|P^m Q^n|\Gamma\rangle, \tag{92b}$$

and we write them in terms of f_{mn} as

$$\tfrac{1}{4}(f_{m+1,n} + f_{m-1,n} + \omega^m f_{m,n+1} + \omega^{-m} f_{m,n-1}) = h f_{m,n}, \tag{93a}$$

$$\tfrac{1}{4}(\omega^n f_{m+1,n} + \omega^{-n} f_{m-1,n} + f_{m,n+1} + f_{m,n-1}) = h f_{m,n}. \tag{93b}$$

Regarding $f_{m,n}$ as the (m,n) entry of the vector $|f\rangle$ in $\mathbb{C}^d \otimes \mathbb{C}^d$, we write Eqs. (93) in the form

$$\mathcal{H}_L\,|f\rangle = h\,|f\rangle, \tag{94a}$$

$$\mathcal{H}_R\,|f\rangle = h\,|f\rangle, \tag{94b}$$

where

$$\mathcal{H}_L = \tfrac{1}{4}(P^{-1}\otimes\mathbf{1} + P\otimes\mathbf{1} + Q\otimes P^{-1} + Q^{-1}\otimes P), \tag{95a}$$

$$\mathcal{H}_R = \tfrac{1}{4}(P^{-1}\otimes Q + P\otimes Q^{-1} + \mathbf{1}\otimes P^{-1} + \mathbf{1}\otimes P). \tag{95b}$$

Thus, $|f\rangle$ is a simultaneous eigenstate of $\mathcal{H}_L$ and $\mathcal{H}_R$ with eigenvalue h.

Let us see $\mathcal{H}_L$ more closely. Express the space $\mathbb{C}^d \otimes \mathbb{C}^d$ as $\bigoplus_{b=0}^{d-1} V^{(b)}$, where

$$V^{(b)} \equiv \mathrm{Span}\{\left|\Psi_a^{(b)}\right\rangle,\ a = 0,\ldots,d-1\}, \tag{96}$$

$$\left|\Psi_a^{(b)}\right\rangle \equiv |a-b\rangle \otimes |\tilde{b}\rangle. \tag{97}$$

We then observe that each term in $\mathcal{H}_L$ transforms the states $|\Psi_a^{(b)}\rangle$ in the following way:

$$P^{-1}\otimes\mathbf{1}\left|\Psi_a^{(b)}\right\rangle = \left|\Psi_{a-1}^{(b)}\right\rangle,$$
$$P\otimes\mathbf{1}\left|\Psi_a^{(b)}\right\rangle = \left|\Psi_{a+1}^{(b)}\right\rangle,$$
$$Q\otimes P^{-1}\left|\Psi_a^{(b)}\right\rangle = \omega^a\left|\Psi_a^{(b)}\right\rangle,$$
$$Q^{-1}\otimes P\left|\Psi_a^{(b)}\right\rangle = \omega^{-a}\left|\Psi_a^{(b)}\right\rangle.$$

This implies that $\mathcal{H}_L = \bigoplus_{b=0}^{d-1} H$, and h is the maximum eigenvalue of $\mathcal{H}_L$, which is d-fold degenerate. The same thing is true for $\mathcal{H}_R$. Therefore, the maximum eigenvalue of $\mathcal{H}_L + \mathcal{H}_R$ is $2h$, and $|f\rangle$ is one of the associated eigenstates. Thus we obtain

$$(\mathcal{H}_L + \mathcal{H}_R)\,|f\rangle = 2h\,|f\rangle. \tag{98}$$

It is useful to define real quantities g_{mn} as

$$g_{mn} \equiv e^{\frac{2\pi i}{d}\frac{mn}{2}} f_{mn}. \tag{99}$$

g_{mn} is real and has the following symmetries:

$$g_{mn}^* = g_{mn},\ \ g_{mn} = g_{nm},$$
$$g_{m,n} = g_{-m,n} = g_{n,-m}.$$

Note that g_{mn} is not periodic with period d for m and n, rather it satisfies the following relations:

$$g_{m\pm d,n} = (-)^n g_{m,n},\ \ g_{m,n\pm d} = (-)^m g_{m,n}.$$

B. $\langle\Gamma|P^m Q^n|\Gamma\rangle \neq 0$ when d is odd

In this subsection, we assume that d is odd, and we fix the range of the indices m, n, m', n' as

$$-(d-1)/2 \leqslant m, n, m', n' \leqslant (d-1)/2. \tag{100}$$

We will show that g_{mn} are strictly positive. Rewriting Eq. (98), we obtain the eigenequation for $|g\rangle \in \mathbb{C}^d \otimes \mathbb{C}^d$ with $\langle mn|g\rangle = g_{mn}$,

$$\mathcal{K}\,|g\rangle = 2h\,|g\rangle, \tag{101}$$

where

$$\mathcal{K}_{mn,m'n'} = e^{\frac{2\pi i}{d}\frac{mn}{2}}(\mathcal{H}_L + \mathcal{H}_R)_{mn,m'n'}\,e^{-\frac{2\pi i}{d}\frac{m'n'}{2}}.$$

We find that $\mathcal{K}_{mn,m'n'}$ is given by

$$\mathcal{K}_{mn,m'n'} = \frac{1}{2}D_{mm'}[(-1)^n]\cos\left(\frac{\pi n}{d}\right)\delta_{nn'} + \frac{1}{2}\cos\left(\frac{\pi m}{d}\right)\delta_{mm'}D_{nn'}[(-1)^m],$$

where the $d\times d$ matrix $D(\sigma)$ is defined as

$$D_{mm'}(\sigma) = \delta_{|m-m'|,1} + \sigma(\delta_{m,(d-1)/2}\delta_{m',-(d-1)/2} + \delta_{m,-(d-1)/2}\delta_{m',(d-1)/2})$$

or

$$D(\sigma) = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & \sigma \\ 1 & 0 & 1 & \ddots & 0 & 0 \\ 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 & 0 \\ 0 & 0 & \ddots & 1 & 0 & 1 \\ \sigma & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

Note that $\cos(\frac{\pi n}{d})$ and $\cos(\frac{\pi m}{d})$ are positive since the ranges of m, n are given by Eq. (100). However, the Perron-Frobenius theorem is not yet applicable to $\mathcal{K}$, since the nondiagonal elements may be negative depending on the even-oddness of m, n.

Here, we notice that $\mathcal{K}$ has the following reflection symmetries:

$$\mathcal{K}_{m,n,m',n'} = \mathcal{K}_{-m,n,-m',n'} = \mathcal{K}_{m,-n,m',-n'}, \tag{102}$$

and g_{mn} is also symmetric under these reflections. To exploit this fact, we rewrite the eigenequation $\mathcal{K}|g\rangle = 2h|g\rangle$ in the base $\{|e_{a,b}\rangle,\ a, b = 0, 1, \ldots, (d-1)/2\}$, which respects the reflection symmetries,

$$|e_{ab}\rangle \equiv |e_a\rangle \otimes |e_b\rangle, \tag{103}$$

$$|e_a\rangle \equiv \frac{1}{\sqrt{2(1+\delta_{a0})}}(|a\rangle + |-a\rangle). \tag{104}$$

In this base, the eigenequation reads

$$\mathcal{K}^{(S)} g^{(S)} = 2h g^{(S)}, \tag{105}$$

where

$$g^{(S)}_{ab} = \langle e_{ab}|g\rangle \tag{106}$$

and

$$\mathcal{K}^{(S)}_{ab,a'b'} = \langle e_{ab}|\mathcal{K}|e_{a'b'}\rangle = \frac{1}{2} D^{(S)}_{aa'}[(-1)^b] \cos\left(\frac{\pi b}{d}\right)\delta_{bb'} + \frac{1}{2}\cos\left(\frac{\pi a}{d}\right)\delta_{aa'} D^{(S)}_{bb'}[(-1)^a]. \tag{107}$$

Here, the $(d+1)/2 \times (d+1)/2$ matrix $D^{(S)}(\sigma)$ is given by

$$D^{(S)}_{aa'}(\sigma) = \langle e_a|D(\sigma)|e_{a'}\rangle = \sqrt{1+\delta_{a,0}}\,\delta_{a,a'-1} + \sqrt{1+\delta_{a',0}}\,\delta_{a',a-1} + \sigma\,\delta_{a,(d-1)/2}\delta_{a',(d-1)/2}$$

or

$$D^{(S)}(\sigma) = \begin{bmatrix} 0 & \sqrt{2} & 0 & \cdots & 0 \\ \sqrt{2} & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \ldots & 0 & 1 & \sigma \end{bmatrix}.$$

Now we examine the real symmetric matrix $\mathcal{K}^{(S)} + \mathbf{1}$. All elements are non-negative, and the diagonal elements are strictly positive. Further, the matrix elements $(\mathcal{K}^{(S)} + \mathbf{1})_{ab,a'b'}$ are strictly positive if the points (a, b) and (a', b') are the nearest neighbors on the two-dimensional integer lattice. Therefore, all elements of $A \equiv (\mathcal{K}^{(S)} + \mathbf{1})^{d-1}$ are strictly positive. Evidently, $g^{(S)}$ is the eigenvector of A with the maximum eigenvalue $(2h+1)^{d-1}$. According to the theorem of Perron-Frobenius, all components of $g^{(S)}$ can be taken to be strictly positive. This further implies that all g_{mn} are strictly positive because of the reflection invariance of g_{mn}. Thus we have shown that $\langle\Gamma|P^m Q^n|\Gamma\rangle \neq 0$ when d is odd.

VI. SUMMARY AND CONCLUDING REMARKS

The aim of this paper is to construct the minimum-uncertainty states and the non-negative quasiprobability distribution for a qudit. They are the finite-dimensional counterparts of the coherent states and the Husimi function of the continuous quantum mechanics.

We reexamined the theorem of Massar and Spindel for the uncertainty relation of the two unitary operators related by the discrete Fourier transformation, and we showed that some assumptions in their proof can be justified if we use the Perron-Frobenius theorem. The minimum-uncertainty states are the ones that saturate this uncertainty inequality. By introducing a scale factor in the continuum limit, we showed that they approach the coherent states with different widths.

We constructed the non-negative quasiprobability distribution, of which marginal distributions are smeared out as in the Husimi function. However, this quasiprobability distribution is shown to be optimal in the sense that there does not exist a non-negative and translationally covariant quasiprobability distribution with sharper marginal properties. Generally, the completeness is one of the desirable properties of a quasiprobability distribution; that is, it contains full information of the state. We showed that the obtained quasiprobability is indeed complete if the dimension of the state space is odd, whereas it is unfortunately not if the dimension is even. It is well known that the Wigner function in the even-dimensional case is much more involved than in the odd-dimensional case (see, e.g., [25,26]). Further investigation for this even-odd issue of quasiprobabilities is certainly needed.

The Wigner function may take negative values. In Refs. [24,27], however, it is shown that one can define non-negative quasiprobabilities by introducing an auxiliary variable into the Wigner function, and solve the dynamics of a quantum system stochastically. It will be of interest in future studies to apply our quasiprobability distribution to this line of research.

[1] W. Heisenberg, Z. Phys. **43**, 172 (1927).
[2] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
[3] C. H. Bennett and G. Brassard, in *Proceedings of IEEE International Conference on Computers, Systems and Signal Processing, Banglore, India, 1984* (IEEE, New York, 1984), pp. 175-179.
[4] W. K. Wootters and W. H. Zurek, Nature (London) **299**, 802 (1982).
[5] E. H. Kennard, Z. Phys. **44**, 326 (1927).
[6] J. R. Klauder and B. S. Skagerstam, *Coherent States: Applications in Physics and Mathematical Physics* (World Scientific, Singapore, 1985).
[7] K. Husimi, Proc. Phys. Math. Soc. Jpn. **22**, 264 (1940).
[8] E. Wigner, Phys. Rev. **40**, 749 (1932).
[9] R. L. Hudson, Rep. Math. Phys. **6**, 249 (1974).
[10] T. Opatrný, V. Bužek, J. Bajer, and G. Drobný, Phys. Rev. A **52**, 2419 (1995).
[11] T. Opatrný, D.-G. Welsch, and V. Bužek, Phys. Rev. A **53**, 3822 (1996).
[12] S. Massar and P. Spindel, Phys. Rev. Lett. **100**, 190401 (2008).
[13] A. B. Klimov, C. Muñoz, and L. L. Sánchez-Soto, Phys. Rev. A **80**, 043836 (2009).
[14] N. Cotfas and D. Dragoman, J. Phys. A **45**, 425305 (2012).
[15] M. A. Marchiolli and M. Ruzzi, Ann. Phys. (NY) **327**, 1538 (2012).
[16] R. A. Horn and C. R. Johnson, *Matrix Analysis* (Cambridge University Press, New York, 1985).
[17] L. Barker, C. Candan, T. Hakioğlu, M. Kutay, and H. M. Ozaktas, J. Phys. A **33**, 2209 (2000).
[18] M. A. Marchiolli and P. E. M. F. Mendonça, Ann. Phys. (NY) **336**, 76 (2013).
[19] B. W. Dickinson and K. Steiglitz, IEEE Trans. Acoust. Speech Sign. Proc. **30**, 25 (1982).
[20] M. Horibe, A. Takami, T. Hashimoto, and A. Hayashi, Phys. Rev. A **65**, 032105 (2002).
[21] D. Gross, J. Math. Phys. **47**, 122107 (2006); Appl. Phys. B **86**, 367 (2007).
[22] M. Horibe, T. Hashimoto, and A. Hayashi, arXiv:1301.7541.
[23] W. K. Wootters, Ann. Phys. (NY) **176**, 1 (1987).
[24] O. Cohendet, Ph. Combe, M. Sirugue, and M. Sirugue-Collin, J. Phys. A **21**, 2875 (1988).
[25] U. Leonhardt, Phys. Rev. Lett. **74**, 4101 (1995); Phys. Rev. A **53**, 2998 (1996).
[26] A. Takami, T. Hashimoto, M. Horibe, and A. Hayashi, Phys. Rev. A **64**, 032114 (2001).
[27] T. Hashimoto, M. Horibe, and A. Hayashi, J. Phys. A **40**, 14253 (2007).