Classification of incompatibility for two orthonormal bases

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For two orthonormal bases of a d-dimensional complex Hilbert space, the notion of complete incompatibility was introduced recently by De Bièvre, [Phys. Rev. Lett. **127**, 190404 (2021)]. In this paper, we introduce the notion of s-order incompatibility with positive integer s satisfying $2 \leqslant s \leqslant d+1$. In particular, $(d+1)$-order incompatibility just coincides with the complete incompatibility. We establish some relations between s-order incompatibility, minimal support uncertainty, and rank deficiency of the transition matrix. As an example, we determine the incompatibility order of the discrete Fourier transform with any finite dimension.

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I. INTRODUCTION

Quantum physics manifests many properties different from classical physics; these properties are called quantum nonclassicality. There are diverse aspects and notions of quantum nonclassicality, such as noncommutativity of two operators, entanglement, coherence, uncertainty principles, nonreality, contextuality, and nonlocality. These nonclassical properties remarkably deepened the understanding of quantum physics and provided fruitful applications in quantum technology.

Suppose $A=\{|a_j\rangle\}_{j=1}^d, B=\{|b_k\rangle\}_{k=1}^d$ are two orthonormal bases of a d-dimensional complex Hilbert space H. To avoid the freedom $|a_j\rangle \to e^{i\theta_j}|a_j\rangle$ with $\theta_j \in R$ (real numbers) and $i=\sqrt{-1}$, we denote $\overline{A}=\{|a_j\rangle\langle a_j|\}_{i=1}^d$ and $\overline{B}=\{|b_k\rangle\langle b_k|\}_{k=1}^d$; that is, $\overline{A}$ and $\overline{B}$ are all rank-1 projective measurements. We adopt the notion of "incompatibility" as in Ref. [1]: When $\overline{A}$ and $\overline{B}$ commute, we say that A and B are compatible; otherwise we say that A and B are incompatible. To say that $\overline{A}$ and $\overline{B}$ commute means that $|a_j\rangle\langle a_j|$ and $|b_k\rangle\langle b_k|$ commute for any $j,k \in [\![1,d]\!]$, where $[\![1,d]\!]$ represents the set of consecutive integers $\{j\}_{j=1}^d$. Thus A and B are compatible if and only if (iff) $\overline{A}=\overline{B}$.

The term "incompatible" in the literature usually refers to the meaning that two positive operator-valued measures (POVMs) are not jointly measurable, such as in Refs. [2–12] and recent reviews (see Refs. [13,14]). A POVM D can be expressed by a set of positive semidefinite operators $D=\{D_j\}_{j=1}^m$ which sum to unity. Two POVMs $D=\{D_j\}_{j=1}^m$ and $E=\{E_k\}_{k=1}^n$ are called compatible iff there exists a POVM $G=\{G_{jk}\}_{j=1,}^m{}_{k=1}^n$ such that $\sum_{j=1}^m G_{jk}=E_k$ for any k and $\sum_{k=1}^n G_{jk}=D_j$ for any j. As a special case, when two measurements are two rank-1 projective measurements $(\overline{A},\overline{B})$ above, we can check that $(\overline{A},\overline{B})$ are jointly measurable iff $\overline{A}=\overline{B}$. In this paper, we only consider the incompatibility of two rank-1 projective measurements $(\overline{A},\overline{B})$. Notice that in some works the term "incompatible" may refer to other meanings than joint measurable. For example, in Ref. [15] the notion of compatibility corresponds to commutativity of the measurement operators.

In Ref. [1], De Bièvre introduced the notion of complete incompatibility. Two orthonormal bases $A=\{|a_j\rangle\}_{j=1}^d$, $B=\{|b_k\rangle\}_{k=1}^d$ are completely incompatible if for any nonempty subsets $\varnothing \neq S_A \subseteq A$, $\varnothing \neq S_B \subseteq B$, $|S_A|+|S_B| \leqslant d$, it holds that $\text{span}\{S_A\} \cap \text{span}\{S_B\}=\{0\}$. Here, $|S_A|$ stands for the number of elements in S_A, and $\text{span}\{S_A\}$ is the subspace spanned by S_A over the complex field C. Although the definition of complete incompatibility is purely algebraic, it possesses a physical interpretation in terms of selective projective measurements [16–18]. It is shown that complete incompatibility closely links with the minimal support uncertainty [1], and also, it is useful to characterize the Kirkwood-Dirac nonclassicality [1].

In this paper, we introduce the notion of s-order incompatibility with $s \in [\![2,d+1]\!]$. Under this definition, complete incompatibility is just $(d+1)$-order incompatibility. This paper is organized as follows. In Sec. II, we give the definition of s-order incompatibility and establish a link between it and the minimal support uncertainty. In Sec. III, we characterize s-order incompatibility via the transition matrix of the two orthonormal bases. In Sec. IV, we give examples to illustrate the calculation of incompatibility order. Section V is a brief summary.

II. s-ORDER INCOMPATIBILITY AND MINIMAL SUPPORT UNCERTAINTY

We give the definition of s-order incompatibility and establish a relation between it and the minimal support uncertainty.

Definition 1. s-order incompatibility. Suppose the integer s satisfies $s \in [\![2,d+1]\!]$ and $A=\{|a_j\rangle\}_{j=1}^d$ and $B=\{|b_k\rangle\}_{k=1}^d$ are two orthonormal bases of the d-dimensional complex Hilbert space H. We say that A and B are s-order incompatible if the following conditions hold.

(a) For any $\varnothing \neq S_A \subseteq A$ and $\varnothing \neq S_B \subseteq B$, if $|S_A|+|S_B| < s$, then $\text{span}\{S_A\} \cap \text{span}\{S_B\}=\{0\}$.

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(b) There exist $\varnothing \neq S_A \subseteq A$ and $\varnothing \neq S_B \subseteq B$, such that $|S_A| + |S_B| = s$ and $\text{span}\{S_A\} \cap \text{span}\{S_B\} \neq \{0\}$.

We use χ_{AB} to denote the incompatibility order of A and B. When $\chi_{AB} = d+1$, the $(d+1)$-order incompatibility just coincides with the complete incompatibility introduced in Ref. [1].

We establish a link between s-order incompatibility and the minimal support uncertainty. For a pure state $|\psi\rangle$, we express it in the orthonormal bases $A = \{|a_j\rangle\}_{j=1}^d$ and $B = \{|b_k\rangle\}_{k=1}^d$ as $|\psi\rangle = \sum_{j=1}^d |a_j\rangle\langle a_j|\psi\rangle$ and $|\psi\rangle = \sum_{k=1}^d |b_k\rangle\langle b_k|\psi\rangle$. We use $n_A(|\psi\rangle)$ to denote the number of nonzero elements in $\{\langle a_j|\psi\rangle\}_{j=1}^d$, use $n_B(|\psi\rangle)$ to denote the number of nonzero elements in $\{\langle b_k|\psi\rangle\}_{k=1}^d$, and let

$$n_{AB}(|\psi\rangle) := n_A(|\psi\rangle) + n_B(|\psi\rangle), \tag{1}$$

$$n_{AB}^{\min} := \min_{|\psi\rangle \neq 0} n_{AB}(|\psi\rangle). \tag{2}$$

$n_{AB}(|\psi\rangle)$ is called the support uncertainty of $|\psi\rangle$ with respect to A and B, and $n_{AB}^{\min}$ is called the minimal support uncertainty with respect to A and B. The support uncertainty $n_{AB}(|\psi\rangle)$ has many applications in different situations [19–23]. Obviously, $n_{AB}^{\min} \in [\![2, d+1]\!]$. It is shown that $\chi_{AB} = d+1$ iff $n_{AB}^{\min} = d+1$ [1]. We now prove a more general result in Theorem 1.

Theorem 1. Suppose $A = \{|a_j\rangle\}_{j=1}^d$ and $B = \{|b_k\rangle\}_{k=1}^d$ are two orthonormal bases of the d-dimensional complex Hilbert space H. The incompatibility order χ_{AB} and minimal support uncertainty $n_{AB}^{\min}$ are defined in Definition 1 and Eq. (2); then it holds that

$$\chi_{AB} = n_{AB}^{\min}. \tag{3}$$

Proof. By the definition of $n_{AB}^{\min}$, if $n_{AB}^{\min} = s$, then there exists a pure state $|\psi\rangle$ such that $n_{AB}(|\psi\rangle) = n_A(|\psi\rangle) + n_B(|\psi\rangle) = s$ and there does not exist a pure state $|\psi'\rangle$ such that $n_{AB}(|\psi'\rangle) = n_A(|\psi'\rangle) + n_B(|\psi'\rangle) < s$. For such $|\psi\rangle$, there exist $\varnothing \neq S_A \subseteq A$ and $\varnothing \neq S_B \subseteq B$, such that $|S_A| = n_A(|\psi\rangle)$, $|S_B| = n_B(|\psi\rangle)$, and $|\psi\rangle \in \text{span}\{S_A\} \cap \text{span}\{S_B\}$. The nonexistence of such $|\psi'\rangle$ implies that there does not exist $\varnothing \neq S_A \subseteq A$ and $\varnothing \neq S_B \subseteq B$, such that $|S_A| = n_A(|\psi'\rangle)$, $|S_B| = n_B(|\psi'\rangle)$, and $|\psi'\rangle \in \text{span}\{S_A\} \cap \text{span}\{S_B\}$. These two conditions just coincide with conditions (a) and (b) in Definition 1. Then the claim follows. ■

Again, when $s = d+1$, Theorem 1 returns to the corresponding result in Ref. [1].

III. s-ORDER INCOMPATIBILITY AND THE TRANSITION MATRIX

In this section, we introduce the index of rank deficiency τ_{AB}. We also establish a link between χ_{AB} ($n_{AB}^{\min}$) and τ_{AB}; then χ_{AB} can be determined via τ_{AB}.

For two orthonormal bases $A = \{|a_j\rangle\}_{j=1}^d$ and $B = \{|b_k\rangle\}_{k=1}^d$, the transition matrix $U^{AB} = (U_{jk}^{AB})_{j,k=1}^d$ is defined as $U_{jk}^{AB} = \langle a_j|b_k\rangle$. Conversely, for a given unitary matrix U, we can always find two orthonormal bases $A = \{|a_j\rangle\}_{j=1}^d$ and $B = \{|b_k\rangle\}_{k=1}^d$ such that $U_{jk} = \langle a_j|b_k\rangle$. For example, when we express $U = (U_{jk})_{j,k=1}^d$ in the standard computational basis $\{|j\rangle\}_{j=1}^d$, let A be this standard computational basis and B be the column vectors of $U = (U_{jk})_{j,k=1}^d$. Note that $U_{jk}^{AB} = \langle a_j|b_k\rangle = \langle a_j|V^\dagger V|b_k\rangle$ for any $d \times d$ unitary matrix V with $V^\dagger$ being the Hermitian conjugate of V; then the transition matrix U with respect to (A, B) is invariant under the unitary operation $V : (A, B) \to (VA, VB)$. Here, $VA = \{V|a_j\rangle\}_{j=1}^d$.

We want to characterize s-order incompatibility via the transition matrix U^{AB}. To do this, we introduce the definition of t-order rank deficiency of U^{AB}.

Definition 2. t-order rank deficiency of U^{AB}. For the transition matrix U^{AB} and the integer $t \in [\![0, d-1]\!]$, we define the t-order rank deficiency of U^{AB} as follows.

$$R_{t,r}(U^{AB}) = \max_{\substack{1\leqslant m\leqslant d-t;\\ 1\leqslant j_1<j_2<\cdots<j_m\leqslant d;\\ 1\leqslant k_1<k_2<\cdots<k_{m+t}\leqslant d}} \left\{ m - \text{rank}\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t}. \end{pmatrix} \right\}, \tag{4}$$

$$R_{t,c}(U^{AB}) = \max_{\substack{1\leqslant m\leqslant d-t;\\ 1\leqslant j_1<j_2<\cdots<j_m\leqslant d;\\ 1\leqslant k_1<k_2<\cdots<k_{m+t}\leqslant d}} \left\{ m - \text{rank}\begin{pmatrix} k_1, k_2, \ldots, k_{m+t}; \\ j_1, j_2, \ldots, j_m. \end{pmatrix} \right\}, \tag{5}$$

$$R_t(U^{AB}) = \max\{R_{t,r}(U^{AB}), R_{t,c}(U^{AB})\}, \tag{6}$$

where $\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t}. \end{pmatrix}$ denotes the submatrix obtained by the $(j_1, j_2, \ldots, j_m)$ rows and $(k_1, k_2, \ldots, k_{m+t})$ columns of U^{AB}, for example, $\begin{pmatrix} 1,3; \\ 2,3,4. \end{pmatrix} = \begin{pmatrix} \langle a_1|b_2\rangle & \langle a_1|b_3\rangle & \langle a_1|b_4\rangle \\ \langle a_3|b_2\rangle & \langle a_3|b_3\rangle & \langle a_3|b_4\rangle \end{pmatrix}$.

Clearly, the definitions of $R_{t,r}(U^{AB})$, $R_{t,c}(U^{AB})$, and $R_t(U^{AB})$ above can be similarly defined for general matrices, not only the unitary matrices. Note that a similar definition of rank-deficient submatrices was proposed in Ref. [24].

Proposition 1. Suppose $t \in [\![0, d-1]\!]$; then the following conditions hold.

(i) $R_t(U^{AB}) \geqslant 0$.

(ii) $0 \leqslant R_t(U^{AB}) - R_{t+1}(U^{AB}) \leqslant 1$.

(iii) $R_{d-1}(U^{AB}) = 0$.

(iv) If $R_0(U^{AB}) = 0$, then $R_t(U^{AB}) = 0$ for any $t \in [\![0, d-1]\!]$.

Proof. Recall that the matrix rank is defined as the rank of row vectors, which also equals the rank of column vectors; then $R_t(U^{AB}) \geqslant 0$ evidently holds since $m \geqslant \text{rank}\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t}. \end{pmatrix}$ and $m \geqslant \text{rank}\begin{pmatrix} k_1, k_2, \ldots, k_{m+t}; \\ j_1, j_2, \ldots, j_m. \end{pmatrix}$.

For $t+1$, according to Definition 2, there exist $1 \leqslant m \leqslant d-(t+1)$ and $\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t+1}. \end{pmatrix}$ such that $R_{t+1}(U^{AB}) = m - \text{rank}\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t+1}. \end{pmatrix}$, or there exist $1 \leqslant n \leqslant (t+1)$ and $\begin{pmatrix} k_1, k_2, \ldots, k_{n+t+1}; \\ j_1, j_2, \ldots, j_n. \end{pmatrix}$ such that $R_{t+1}(U^{AB}) = n - \text{rank}\begin{pmatrix} k_1, k_2, \ldots, k_{n+t+1}; \\ j_1, j_2, \ldots, j_n. \end{pmatrix}$. We consider the former case; the latter can be discussed similarly. For the former case, we see that

$$\begin{aligned} R_{t+1}(U^{AB}) &= m - \text{rank}\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t+1}. \end{pmatrix} \\ &\leqslant (m+1) - \text{rank}\begin{pmatrix} l_1, l_2, \ldots, l_m, l_{m+1}; \\ k_1, k_2, \ldots, k_{m+t+1}. \end{pmatrix} \\ &\leqslant R_t(U^{AB}), \end{aligned}$$

where $0 < l_1 < l_2 < \cdots < l_m < l_{m+1} \leqslant d$ and $\{j_1, j_2, \ldots, j_m\} \subseteq \{l_1, l_2, \ldots, l_m, l_{m+1}\}$. The first inequality states the fact that adding one row can at most increase the rank by 1. The second inequality is from the definition of $R_t(U^{AB})$. Then $R_t(U^{AB}) \geqslant R_{t+1}(U^{AB})$.

When $t = d-1$, from Definition 2, m can only take $m = 1$. Since U^{AB} is unitary, then every row vector and every column vector of U^{AB} is nonzero. Hence $R_{d-1}(U^{AB}) = 0$. This proves condition (iii).

Condition (iv) is a direct result of $R_t(U^{AB}) \geqslant R_{t+1}(U^{AB})$ and condition (iii).

Lastly, we prove $R_t(U^{AB}) - R_{t+1}(U^{AB}) \leqslant 1$. If $R_t(U^{AB}) \leqslant 1$, then the claim is obviously true. Suppose $R_t(U^{AB}) \geqslant 2$ and the submatrix $\binom{j_1, j_2, \ldots, j_m;}{k_1, k_2, \ldots, k_{m+t}.}$ reaches $R_t(U^{AB}) = m - \operatorname{rank}\binom{j_1, j_2, \ldots, j_m;}{k_1, k_2, \ldots, k_{m+t}.}$; we see that $m \geqslant 2$. Removing any row, the remaining submatrix, for example, is $\binom{j_1, j_2, \ldots, j_{m-1};}{k_1, k_2, \ldots, k_{m+t}.}$. We have that

$$\begin{aligned} R_{t+1}(U^{AB}) &\geqslant (m-1) - \operatorname{rank}\begin{pmatrix} j_1, j_2, \ldots, j_{m-1}; \\ k_1, k_2, \ldots, k_{m+t}. \end{pmatrix} \\ &\geqslant m - \operatorname{rank}\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+t}. \end{pmatrix} - 1 \\ &= R_t(U^{AB}) - 1; \end{aligned}$$

then condition (ii) is true, and we finish this proof. ■

With Proposition 1, we propose the definition of the index of rank deficiency of the transition matrix U^{AB}.

Definition 3. We define the index of rank deficiency of the transition matrix U^{AB} as

$$\tau_{AB} := \min_{t \in [\![0, d-1]\!]} \{t | R_t(U^{AB}) = 0\} - 1. \tag{7}$$

Clearly, $\tau_{AB} \in [\![-1, d-2]\!]$. When $R_0(U^{AB}) = 0$, we have that $\tau_{AB} = -1$. For $\tau_{AB} = -1$, every $m \times m$ submatrix $\binom{j_1, j_2, \ldots, j_m;}{k_1, k_2, \ldots, k_m.}$ is of rank m, particularly, every element $U^{AB}_{jk} = \langle a_j | b_k \rangle \neq 0$. When $\tau_{AB} \in [\![0, d-2]\!]$, τ_{AB} is the maximal t for which $R_t(U^{AB}) > 0$; for such a case it must hold that $R_{\tau_{AB}}(U^{AB}) = 1$. Hence we have Corollary 1 below.

Corollary 1. Suppose $\tau_{AB} \in [\![0, d-2]\!]$; then $R_{\tau_{AB}}(U^{AB}) = 1$, and

$$\tau_{AB} = \max_{t \in [\![0, d-1]\!]} \{t | R_t(U^{AB}) = 1\}. \tag{8}$$

If $\binom{j_1, j_2, \ldots, j_m;}{k_1, k_2, \ldots, k_{m+\tau_{AB}}.}$ reaches $R_{\tau_{AB}}(U^{AB}) = 1$, we assert that there must exist $\{z_j\}_{j=1}^m$ that are complex numbers and all nonzero such that

$$(z_1, z_2, \ldots, z_m)\begin{pmatrix} j_1, j_2, \ldots, j_m; \\ k_1, k_2, \ldots, k_{m+\tau_{AB}}. \end{pmatrix} = 0. \tag{9}$$

Otherwise, if $\{z_j\}_{j=1}^m$ are not all nonzero, for example, $\{z_j \neq 0\}_{j=1}^{m-1}$ and $z_m = 0$, then Eq. (9) implies that $\binom{j_1, j_2, \ldots, j_{m-1};}{k_1, k_2, \ldots, k_{m+\tau_{AB}}.}$ is rank deficient in rows and $R_{\tau_{AB}+1}(U^{AB}) \geqslant 1$; this contradicts Eq. (8).

Similarly, if $\binom{k_1, k_2, \ldots, k_{n+\tau_{AB}};}{j_1, j_2, \ldots, j_n.}$ reaches $R_{\tau_{AB}}(U^{AB}) = 1$, then there exist $\{z_j\}_{j=1}^n$ that are complex numbers and all nonzero such that

$$\begin{pmatrix} k_1, k_2, \ldots, k_{n+\tau_{AB}}; \\ j_1, j_2, \ldots, j_n. \end{pmatrix}(z_1, z_2, \ldots, z_n)^t = 0, \tag{10}$$

where $(\ )^t$ denotes the transpose.

In Ref. [1], it is shown that when A and B are completely incompatible, i.e., $\chi_{AB} = d+1$, then it holds that $\tau_{AB} = -1$. Theorem 2 below shows a more general result, which is the central result of this work.

Theorem 2. Suppose $A = \{|a_j\rangle\}_{j=1}^d$ and $B = \{|b_j\rangle\}_{j=1}^d$ are two orthonormal bases of the d-dimensional complex Hilbert space H. Then the incompatibility order χ_{AB} and the index of rank deficiency τ_{AB} have the relation

$$\chi_{AB} + \tau_{AB} = d. \tag{11}$$

Proof. The case of $\chi_{AB} = d+1$ has been proved in Ref. [1]; therefore we only consider the case of $2 \leqslant \chi_{AB} \leqslant d$. Suppose the incompatibility order is χ_{AB}; then condition (b) in Definition 1 holds, that is, there exist $\varnothing \neq S_A \subseteq A$ and $\varnothing \neq S_B \subseteq B$ such that $|S_A| + |S_B| = \chi_{AB}$ and $\operatorname{span}\{S_A\} \cap \operatorname{span}\{S_B\} \neq \{0\}$. Then there exists a pure state $|\psi\rangle \in \operatorname{span}\{S_A\} \cap \operatorname{span}\{S_B\}$. Without loss of generality, we assume $S_A = \{|a_j\rangle\}_{j=1}^{|S_A|}$, $S_B = \{|b_k\rangle\}_{k=1}^{|S_B|}$. We explicitly write U^{AB} as

$$\begin{pmatrix} \langle a_1|b_1\rangle & \cdots & \langle a_1|b_{|S_B|}\rangle & \langle a_1|b_{|S_B|+1}\rangle & \cdots & \langle a_1|b_d\rangle \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \langle a_{|S_A|}|b_1\rangle & \cdots & \langle a_{|S_A|}|b_{|S_B|}\rangle & \langle a_{|S_A|}|b_{|S_B|+1}\rangle & \cdots & \langle a_{|S_A|}|b_d\rangle \\ \langle a_{|S_A|+1}|b_1\rangle & \cdots & \langle a_{|S_A|+1}|b_{|S_B|}\rangle & \langle a_{|S_A|+1}|b_{|S_B|+1}\rangle & \cdots & \langle a_{|S_A|+1}|b_d\rangle \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \langle a_d|b_1\rangle & \cdots & \langle a_d|b_{|S_B|}\rangle & \langle a_d|b_{|S_B|+1}\rangle & \cdots & \langle a_d|b_d\rangle \end{pmatrix}. \tag{12}$$

Expanding $|\psi\rangle$ in S_A and S_B, we get that

$$|\psi\rangle = \sum_{j=1}^{|S_A|} x_j |a_j\rangle = \sum_{k=1}^{|S_B|} y_k |b_k\rangle,$$

where $\{x_j\}_{j=1}^{S_A}$ are all nonzero complex numbers and $\{y_k\}_{k=1}^{S_B}$ are all nonzero complex numbers. $x_j = 0$ or $y_k = 0$ will contradict $|S_A| + |S_B| = \chi_{AB} = n_{AB}^{\min}$. Consequently,

$$\langle \psi | b_k \rangle = 0 \quad \text{for all } |S_B| + 1 \leqslant k \leqslant d,$$

$$\langle a_j | \psi \rangle = 0 \quad \text{for all } |S_A| + 1 \leqslant j \leqslant d.$$

These imply that

$$\sum_{j=1}^{|S_A|} x_j^* \langle a_j|b_k\rangle = 0 \quad \text{for all } |S_B|+1 \leqslant k \leqslant d,$$

$$\sum_{k=1}^{|S_B|} y_k \langle a_j|b_k\rangle = 0 \quad \text{for all } |S_A|+1 \leqslant j \leqslant d,$$

where x_j^* is the complex conjugate of x_j. These say that the $|S_A| \times (d - |S_B|)$ submatrix $\binom{1,2,\ldots,|S_A|;}{|S_B|+1,|S_B|+2,\ldots,d.}$ has linearly dependent row vectors and the $(d - |S_A|) \times |S_B|$ submatrix $\binom{|S_A|+1,|S_A|+2,\ldots,d;}{1,2,\ldots,|S_B|.}$ has linearly dependent column vectors. Since $2 \leqslant \chi_{AB} \leqslant d$, then $|S_A| + |S_B| \leqslant d$, $|S_A| \leqslant d - |S_B|$, and $|S_B| \leqslant d - |S_A|$. These further imply that $R_{d-|S_A|-|S_B|}(U^{AB}) > 0$ and $\tau_{AB} \geqslant d - \chi_{AB}$.

Conversely, suppose the index of rank deficiency is τ_{AB}; then there exist $1 \leqslant m \leqslant d - \tau_{AB}$ and $\binom{j_1,j_2,\ldots,j_m;}{k_1,k_2,\ldots,k_{m+\tau_{AB}}.}$ such that $m - \text{rank}\binom{j_1,j_2,\ldots,j_m;}{k_1,k_2,\ldots,k_{m+\tau_{AB}}.} = 1$, or there exist $1 \leqslant n \leqslant d - \tau_{AB}$ and $\binom{k_1,k_2,\ldots,k_{n+\tau_{AB}};}{j_1,j_2,\ldots,j_n.}$ such that $n - \text{rank}\binom{k_1,k_2,\ldots,k_{n+t_2};}{j_1,j_2,\ldots,j_n.} = 1$. We consider the former case; the latter can be discussed similarly. For the former case, without loss of generality, we assume that $\binom{j_1,j_2,\ldots,j_m;}{k_1,k_2,\ldots,k_{m+\tau_{AB}}.} = \binom{1,2,\ldots,m;}{1,2,\ldots,m+\tau_{AB}.}$. Since $m - \text{rank}\binom{1,2,\ldots,m;}{1,2,\ldots,m+\tau_{AB}.} = 1$, then there must exist $\{z_j\}_{j=1}^m$ that are complex numbers and all nonzero such that

$$\sum_{j=1}^{m} z_j \langle a_j|b_k\rangle = 0 \quad \text{for all } 1 \leqslant k \leqslant m + \tau_{AB}.$$

Let $|\varphi\rangle = \sum_{j=1}^m z_j^* |a_j\rangle$; then $|\varphi\rangle \neq 0$ and

$$\langle \varphi|b_k\rangle = 0 \quad \text{for all } 1 \leqslant k \leqslant m + \tau_{AB}.$$

It follows that $n_A(|\varphi\rangle) = m$, $n_B(|\varphi\rangle) \leqslant d - m - \tau_{AB}$, and

$$\chi_{AB} = n_{AB}^{\min} \leqslant n_A(|\varphi\rangle) + n_B(|\varphi\rangle) \leqslant d - \tau_{AB}.$$

Theorem 2 then follows. ■

Theorem 2 and Theorem 1 provide a way to determine χ_{AB} and $n_{AB}^{\min}$ via τ_{AB}. From the proof of Theorem 2, we see that there exist $\binom{j_1,j_2,\ldots,j_m;}{k_1,k_2,\ldots,k_{m+1}.}$ and $\binom{k_1,k_2,\ldots,k_{n+1};}{j_1,j_2,\ldots,j_n.}$ such that $m - \text{rank}\binom{j_1,j_2,\ldots,j_m;}{k_1,k_2,\ldots,k_{m+1}.} = n - \text{rank}\binom{k_1,k_2,\ldots,k_{n+1};}{j_1,j_2,\ldots,j_n.} = 1$. We conclude this fact as Corollary 2 below.

Corollary 2. Suppose $\tau_{AB} \in [\![0, d-2]\!]$; then

$$R_{\tau_{AB}}(U^{AB}) = R_{\tau_{AB},r}(U^{AB}) = R_{\tau_{AB},c}(U^{AB}) = 1. \tag{13}$$

IV. EXAMPLES

We give some examples to illustrate the computation of $R_t(U^{AB})$ and incompatibility order.

Example 1. For $d = 6$, we consider $R_t(U^{AB})$ of the unity matrix

$$U^{AB} = I_6 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{14}$$

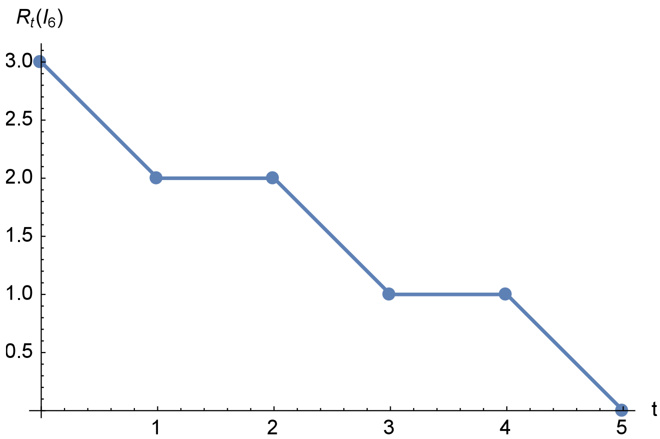

FIG. 1. Plot of $\{R_t(I_6)\}_{t\in[\![0,5]\!]}$ in example 1.

I_6 is symmetric; then $R_t(I_6) = R_{t,r}(I_6) = R_{t,c}(I_6)$. We only need to consider $R_{t,r}(I_6)$. By condition (iii) of Proposition 1, one sees that $R_5(I_6) = 0$.

For $R_4(I_6)$, condition (ii) of Proposition 1 implies that $R_4(I_6) = 0$ or 1. Since the submatrix $\text{rank}\binom{1;}{2,3,4,5,6.} = 0$, then we get $R_4(I_6) = 1$.

For $R_3(I_6)$, condition (ii) of Proposition 1 implies that $R_3(I_6) = 1$ or 2. Since $\text{rank}\binom{j_1;}{k_1,k_2,k_3,k_4.} = 0$ or 1, then $1 - \text{rank}\binom{j_1;}{k_1,k_2,k_3,k_4.} = 0$ or 1. Since $\text{rank}\binom{j_1,j_2,j_3;}{1,2,3,4,5,6.} = 3$, then $3 - \text{rank}\binom{j_1,j_2,j_3;}{1,2,3,4,5,6.} = 0$. Since $\text{rank}\binom{j_1,j_2;}{k_1,k_2,k_3,k_4,k_5.} = 1$ or 2, then $2 - \text{rank}\binom{j_1,j_2,j_3;}{1,2,3,4,5,6.} = 0$ or 1. In conclusion, $R_3(I_6) = 1$.

For $R_2(I_6)$, condition (ii) of Proposition 1 implies that $R_2(I_6) = 1$ or 2. Since $\text{rank}\binom{1,2;}{3,4,5,6.} = 0$ and $2 - \text{rank}\binom{1,2;}{3,4,5,6.} = 2$, then $R_2(I_6) = 2$.

For $R_1(I_6)$, condition (ii) of Proposition 1 implies that $R_1(I_6) = 2$ or 3. Since $\text{rank}\binom{j_1,j_2,j_3;}{k_1,k_2,k_3,k_4.} \in \{1, 2, 3\}$, then $3 - \text{rank}\binom{j_1,j_2,j_3;}{1,2,3,4,5,6.} \in \{0, 1, 2\}$. Since $\text{rank}\binom{j_1,j_2,j_3,j_4;}{k_1,k_2,k_3,k_4,k_5.} = 3$ or 4, then $4 - \text{rank}\binom{j_1,j_2,j_3;}{1,2,3,4,5,6.} = 0$ or 1. Since $\text{rank}\binom{j_1,j_2,j_3,j_4,j_5;}{1,2,3,4,5,6.} = 5$, then $5 - \text{rank}\binom{j_1,j_2,j_3,j_4,j_5;}{1,2,3,4,5,6.} = 0$. In conclusion, $R_1(I_6) = 2$.

For $R_0(I_6)$, condition (ii) of Proposition 1 implies that $R_1(I_6) = 2$ or 3. Since $\text{rank}\binom{1,2,3;}{4,5,6.} = 0$, then $3 - \text{rank}\binom{1,2,3;}{4,5,6.} = 3$; therefore $R_0(I_6) = 3$.

We depict $\{R_t(I_6)\}_{t\in[\![0,5]\!]}$ in Fig. 1. As a result, $\tau_{AB} = 4$, $\chi_{AB} = 2$.

Example 2. For a qubit system, $d = 2$,

$$U^{AB} = \begin{pmatrix} e^{i\varphi_1}\sin\theta & -e^{-i\varphi_2}\cos\theta \\ e^{i\varphi_2}\cos\theta & e^{-i\varphi_1}\sin\theta \end{pmatrix}, \tag{15}$$

where $\theta, \varphi_1, \varphi_2$ are real numbers and $\theta \in [0, \frac{\pi}{2}]$. By condition (iii) of Proposition 1, one sees that $R_1(U^{AB}) = 0$. For $R_0(U^{AB})$, condition (ii) of Proposition 1 implies that $R_0(U^{AB}) = 0$ or 1. When $\theta = 0$ or $\frac{\pi}{2}$, $\sin\theta = 0$ or $\cos\theta = 0$, we have $R_0(U^{AB}) = 1$, $\tau_{AB} = 0$, $\chi_{AB} = 2$, $\overline{A} = \overline{B}$. When $0 \neq \theta \neq \frac{\pi}{2}$, we have $R_0(U^{AB}) = 0$, $\tau_{AB} = -1$, $\chi_{AB} = 3 = d + 1$, and A and B are completely incompatible.

Example 3. For $d=3$, consider the unitary matrix [25]

$$U^{AB}(\theta_1,\theta_2)=\begin{pmatrix}\cos\theta_1\cos\theta_2 & \sin\theta_1 & \cos\theta_1\sin\theta_2\\ -\sin\theta_1\cos\theta_2 & \cos\theta_1 & -\sin\theta_1\sin\theta_2\\ -\sin\theta_2 & 0 & \cos\theta_2\end{pmatrix}, \tag{16}$$

where $\theta_1,\theta_2\in[0,\frac{\pi}{2}]$.

By condition (iii) of Proposition 1, one sees that $R_2(U^{AB})=0$.

For $R_0(U^{AB})$, one sees that since $\mathrm{rank}\binom{1,2,3;}{1,2,3.}=3$, then $3-\mathrm{rank}\binom{1,2,3;}{1,2,3.}=0$. The unitarity of U^{AB} implies that $\mathrm{rank}\binom{j_1,j_2;}{k_1,k_2.}\neq 0$; then $\mathrm{rank}\binom{j_1,j_2;}{k_1,k_2.}=1$ or 2, and therefore $2-\mathrm{rank}\binom{j_1,j_2;}{k_1,k_2.}=0$ or 1. Since $\mathrm{rank}\binom{3;}{2.}=0$, then $1-\mathrm{rank}\binom{3;}{2.}=1$. Consequently, $R_0(U^{AB})=1$.

For $R_1(U^{AB})$, the unitarity of U^{AB} implies that $\mathrm{rank}\binom{j_1,j_2;}{1,2,3.}=2$ and $\mathrm{rank}\binom{1,2,3;}{k_1,k_2.}=2$; then $2-\mathrm{rank}\binom{j_1,j_2;}{1,2,3.}=0$, and $2-\mathrm{rank}\binom{1,2,3;}{k_1,k_2.}=0$. Since $\mathrm{rank}\binom{j_1;}{k_1,k_2.}=0$ or 1, then $\mathrm{rank}\binom{j_1,j_2;}{k_1.}=0$ or 1, and there exists $\mathrm{rank}\binom{j_1;}{k_1,k_2.}=0$ or $\mathrm{rank}\binom{j_1,j_2;}{k_1.}=0$ iff

$$\theta_1=0 \quad\text{or}\quad \theta_1=\frac{\pi}{2} \quad\text{or}\quad \theta_2=0 \quad\text{or}\quad \theta_2=\frac{\pi}{2}. \tag{17}$$

When Eq. (17) holds, then $R_1(U^{AB})=1$; otherwise $R_1(U^{AB})=0$.

It follows that when Eq. (17) holds, then $\tau_{AB}=1$, $\chi_{AB}=2$; otherwise $\tau_{AB}=0$, $\chi_{AB}=3$.

Example 4: Discrete Fourier transform matrix F. $F=U^{AB}$ is defined as $F_{jk}=U^{AB}_{jk}=\langle a_j|b_k\rangle=\frac{1}{\sqrt{d}}e^{i\frac{2\pi}{d}jk}$, with $i=\sqrt{-1}$, $j\in[\![0,d-1]\!]$, $k\in[\![0,d-1]\!]$.

It is shown that A, B are completely incompatible ($\chi_{AB}=d+1$) iff d is a prime [1,21]. We now consider the general case that d is not necessarily a prime. We have Theorem 3 below.

Theorem 3. For a d-dimensional discrete Fourier transform (DFT), it holds that

$$\chi_{AB}=d'+d/d', \tag{18}$$

$$d':=\max\{d_1|d_1|d,\, d_1\leqslant\sqrt{d}\}, \tag{19}$$

where $d_1|d$ means that d_1 is a divisor of d. We will provide a proof for Theorem 3 in the Appendix.

We give another equivalent expression for Eq. (18). Suppose f is a nonzero complex valued function on the index set $\{j\}_{j=0}^{d-1}$; let $\widehat{f}$ denote the DFT of f, that is,

$$\widehat{f}(k)=\frac{1}{\sqrt{d}}\sum_{j=0}^{d-1}e^{i\frac{2\pi}{d}jk}f(j).$$

The support of f, denoted by $\mathrm{supp}f$, is defined as

$$\mathrm{supp}f:=\{j|j\in[\![0,d-1]\!],\, f(j)\neq 0\}.$$

Let the pure state $|\psi\rangle=\sum_{j=0}^{d-1}f(j)|a_j\rangle$; then

$$|\mathrm{supp}f|=n_A(|\psi\rangle).$$

Rewrite $|\psi\rangle=\sum_{j=0}^{d-1}f(j)|a_j\rangle=\sum_{j,k=0}^{d-1}f(j)|b_k\rangle\langle b_k|a_j\rangle=\sum_{j,k=0}^{d-1}F_{kj}f(j)|b_k\rangle=\sum_{j,k=0}^{d-1}\widehat{f}(k)|b_k\rangle$; then

$$|\mathrm{supp}\widehat{f}|=n_B(|\psi\rangle).$$

We then can recast Eq. (18) as an uncertainty principle

$$|\mathrm{supp}f|+|\mathrm{supp}\widehat{f}|\geqslant d'+d/d', \tag{20}$$

and the lower bound on the right-hand side is sharp.

In 1989, Donoho and Stark [19] established an uncertainty principle for $|\mathrm{supp}f|$ and $|\mathrm{supp}\widehat{f}|$ of the DFT, as

$$|\mathrm{supp}f||\mathrm{supp}\widehat{f}|\geqslant d, \tag{21}$$

and the lower bound on the right-hand side is sharp.

In 2005, Tao [21] proved a stronger uncertainty principle of the DFT for $d=p$, where p a prime, as

$$|\mathrm{supp}f|+|\mathrm{supp}\widehat{f}|\geqslant p+1, \tag{22}$$

and the lower bound on the right-hand side is sharp.

We see that our result in Eq. (20) evidently includes Eq. (22) as a special case.

V. SUMMARY

For two orthonormal bases A, B of a quantum system, we introduced the notion of incompatibility order χ_{AB}, which resulted in a classification for incompatibility. We introduced the notion of the index of rank deficiency of the transition matrix U^{AB}, denoted by τ_{AB}. We established a link between χ_{AB} and minimal support uncertainty $n_{AB}^{\min}$ and established a link between χ_{AB} and τ_{AB}. As an application of these relations, we derived the incompatibility order of the DFT.

Note added. Recently, I became aware of a recent work [26] which provides an in-depth study of the complete incompatibility and its links to the support uncertainty and to the Kirkwood-Dirac nonclassicality of pure quantum states.

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APPENDIX: PROOF OF THEOREM 3

When d is a prime, Theorem 3 returns to Eq. (22) in the main text, which has been proved in Ref. [21]. Then we only consider the case that d is not prime. Note that $F=F^t$ and thus $R_{t,r}(F)=R_{t,c}(F)$.

Suppose

$$d=d_1d_2, \tag{A1}$$

with $d_1|d$, $d_2|d$ and $1<d_1\leqslant d_2<d$. We rewrite the index sets $\{j\}_{j=0}^{d-1}$ and $\{k\}_{k=0}^{d-1}$ as

$$j=j_0+j'd_2,\quad j_0\in[\![0,d_2-1]\!],\quad j'\in[\![0,d_1-1]\!], \tag{A2}$$

$$k=k_0+k'd_1,\quad k_0\in[\![0,d_1-1]\!],\quad k'\in[\![0,d_2-1]\!]; \tag{A3}$$

then

$$F_{jk}=\frac{1}{\sqrt{d}}e^{i\frac{2\pi}{d}jk}=\frac{1}{\sqrt{d}}e^{i\frac{2\pi}{d}j_0k_0}e^{i\frac{2\pi}{d}j_0k'd_1}e^{i\frac{2\pi}{d}k_0j'd_2}, \tag{A4}$$

where we have used the fact that $e^{i\frac{2\pi}{d}j'k'd_1d_2}=1$. As pointed out in Ref. [24], Eq. (A4) implies that

$$\mathrm{rank}\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k'\in[\![0,d_2-1]\!]}.\end{pmatrix}=1 \quad (A5)$$

since

$$\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k'\in[\![0,d_2-1]\!]}.\end{pmatrix}=\frac{1}{\sqrt{d}}e^{i\frac{2\pi}{d}j_0k_0}F_{k_0}^tF_{j_0}, \quad (A6)$$

where we have denoted the row vector

$$F_{k_0}=\left(1,e^{i\frac{2\pi}{d}k_0d_2},e^{2i\frac{2\pi}{d}k_0d_2},\dots,e^{(d_1-1)i\frac{2\pi}{d}k_0d_2}\right) \quad (A7)$$

and denoted the transpose of F_{k_0} by $F_{k_0}^t$.

The submatrix $\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k_0\in[\![1,d_1-1]\!],k'\in[\![0,d_2-1]\!]}.\end{pmatrix}$ can be viewed as the column union of the submatrices $\{\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k'\in[\![0,d_2-1]\!]}.\end{pmatrix}\}_{k_0\in[\![1,d_1-1]\!]}$, and thus the column rank (and then the rank)

$$\mathrm{rank}\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k_0\in[\![1,d_1-1]\!],k'\in[\![0,d_2-1]\!]}.\end{pmatrix}\leqslant d_1-1. \quad (A8)$$

Since $\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k_0\in[\![1,d_1-1]\!],k'\in[\![0,d_2-1]\!]}.\end{pmatrix}$ has d_1 rows, thus $\begin{pmatrix}\{j_0+j'd_2\}_{j'\in[\![0,d_1-1]\!]};\\ \{k_0+k'd_1\}_{k_0\in[\![1,d_1-1]\!],k'\in[\![0,d_2-1]\!]}.\end{pmatrix}$ is rank deficient for rows. By the definition of τ_{AB}, it follows that $\tau_{AB}\geqslant(d_1-1)d_2-d_1$, that is

$$\tau_{AB}\geqslant d-(d_1+d_2). \quad (A9)$$

Minimizing d_1+d_2 over all d_1 under Eq. (A1) will yield

$$\tau_{AB}\geqslant d-(d'+d/d'), \quad (A10)$$

$$d':=\max\{d_1|1<d_1\leqslant\sqrt{d},d_1|d\}. \quad (A11)$$

Applying Theorem 2, we see that Eq. (A10) is equivalent to

$$\chi_{AB}\leqslant d'+d/d'. \quad (A12)$$

Next, we prove that $\chi_{AB}\geqslant d'+d/d'$; then Theorem 3 follows. For simplicity of notation, we let $d/d'=d''$.

Lemma 1 (Ref. [27]). Let $d_1<d_2$ be two consecutive divisors of d. If $d_1\leqslant|\mathrm{supp}f|\leqslant d_2$, then

$$|\mathrm{supp}\widehat{f}|\geqslant\frac{d}{d_1d_2}(d_1+d_2-|\mathrm{supp}f|). \quad (A13)$$

Adding $|\mathrm{supp}f|$ to both sides of Eq. (A13), we get

$$|\mathrm{supp}f|+|\mathrm{supp}\widehat{f}|\geqslant\frac{d}{d_1}+\frac{d}{d_2}+\left(1-\frac{d}{d_1d_2}\right)|\mathrm{supp}f|. \quad (A14)$$

Define the function

$$\zeta_d(x)=\frac{d}{d_1(x)}+\frac{d}{d_2(x)}+\left[1-\frac{d}{d_1(x)d_2(x)}\right]x, \quad (A15)$$

where $x\in[1,d]$, $d_1(x)$ is the greatest divisor of d satisfying $d_1(x)\leqslant x$, and $d_2(x)$ is the least divisor of d satisfying $d_2(x)\geqslant x$. If $x=q$, where q a positive integer, and $q|d$, then $d_1(q)=d_2(q)=q$. $\zeta_d(x)$ has the obvious properties below.

(a) $\zeta_d(q)=\zeta_d(\frac{d}{q})=q+\frac{d}{q}$ when $q|d$.

(b) $\zeta_d(x)=d'+d''$, where $x\in[d',d'']$.

(c) $\zeta_d(x)$ is linear with respect to x when $x\in[d_1,d_2]$ and $d_1<d_2$ are two consecutive divisors of d.

(d) The following holds:

$$1-\frac{d}{d_1(x)d_2(x)}<0 \quad \text{when } x\in(1,d')$$
$$1-\frac{d}{d_1(x)d_2(x)}=0 \quad \text{when } x\in(d',d'')$$
$$1-\frac{d}{d_1(x)d_2(x)}>0 \quad \text{when } x\in(d',d]. \quad (A16)$$

Consequently, $\zeta_d(x)$ decreases when x increases in $[1,d']$, $\zeta_d(x)$ increases when x increases in $[d'',d]$, and $\zeta_d(x)$ keeps constant when x increases in $[d',d'']$. It follows that $\zeta_d(x)\geqslant d'+d''$ and the lower bound $d'+d''$ is reached only when $x\in[d',d'']$. Also, $\zeta_d(x)$ is a convex function. When d is a square number, then $d'=d''$, $d=d'^2$, and only one value, $x=d'$, reaches the minimum $\zeta_d(d')=2d'$. When d is not a square number, then $d'<d''$, and all $x\in[d',d'']$ reach the minimum $\zeta_d(d')=\zeta_d(d'')=d'+d''$. We plot $\zeta_{12}(x)$ (12 is not a square number) and $\zeta_{36}(x)$ (36 is a square number) in Figs. 2 and 3.

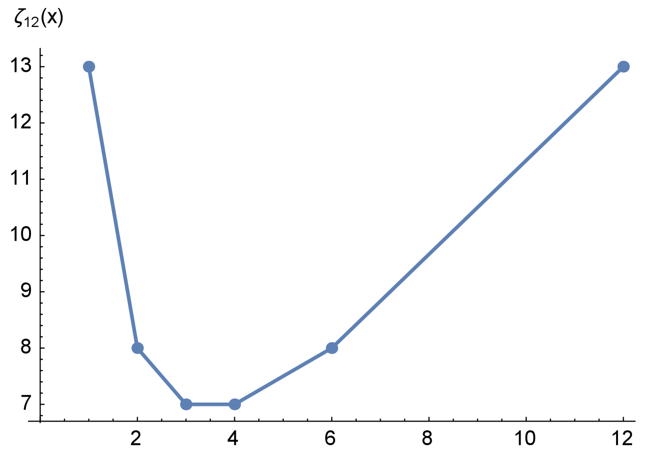

FIG. 2. Plot of $\varsigma_{12}(x)$ in Eq. (A15). All $x\in[3,4]$ reach the minimum $\varsigma_{12}(3)=\varsigma_{12}(4)=7$.

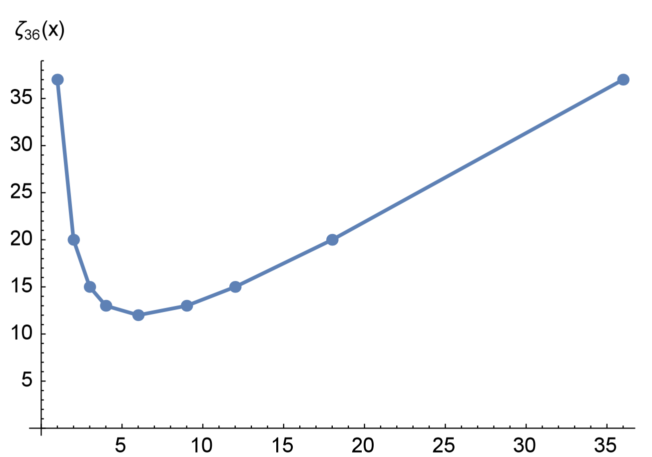

FIG. 3. Plot of $\varsigma_{36}(x)$ in Eq. (A15). Only one value, $x=6$, reaches the minimum $\zeta_d(6)=12$.

Returning to Eq. (A14), we get that

$$|\mathrm{supp} f| + |\mathrm{supp} \widehat{f}| \geqslant d' + d''; \quad \text{(A17)}$$

this certainly implies that

$$\chi_{AB} \geqslant d' + d''. \quad \text{(A18)}$$

Combining Eqs. (A12) and (A18), Theorem 3 then follows.

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