Quantumness of Pure-State Ensembles via Coherence of Gram Matrix Based on Generalized $\alpha$-$z$-Relative Rényi Entropy

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Abstract
The Gram matrix of a set of quantum pure states plays key roles in quantum information theory. It has been highlighted that the Gram matrix of a pure-state ensemble can be viewed as a quantum state, and the quantumness of a pure-state ensemble can thus be quantified by the coherence of the Gram matrix [Europhys. Lett. 134, 30003]. Instead of the $l_1$-norm of coherence and the relative entropy of coherence, we utilize the generalized $\alpha$-$z$-relative Rényi entropy of coherence of the Gram matrix to quantify the quantumness of a pure-state ensemble and explore its properties. We show the usefulness of this quantifier by calculating the quantumness of six important pure-state ensembles. Furthermore, we compare our quantumness with other existing ones and show their features as well as orderings.

Keywords Gram matrix · Quantum ensemble · Quantumness · Generalized $\alpha$-$z$-relative Rényi entropy

1 Introduction
Defined by a finite set of vectors in an inner product space [1], the Gram matrix has been extensively applied in many different branches of mathematics and physics. Notable features of the Gram matrix, including the eigenvalues [2], the trace [3], the determinant [4] and the entropy [5], have been investigated. Recently, it has been shown that many important issues in quantum information theory, such as uncertainty relations [6–8], state discrimination [9–14], transitions between two sets of quantum states [15, 16], information-theoretic aspects of superposition [17], quantum information masking [18] and PT-symmetric quantum systems [19], are intimately related to the Gram matrix.

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On the other hand, the characterization and quantification of the quantumness of ensembles have received extensive attention in the past few years. Various quantifiers of the quantumness of ensembles have been introduced [20–31]. Recently, it is pointed out by Sun, Luo and Lei [32] that the Gram matrix of a pure-state ensemble can be recognized as a quantum state. Based on this observation, a quantification of the quantumness of a pure-state ensemble has been proposed by exploiting the coherence of the Gram matrix of the ensemble.

Motivated by the work [32], in this paper we adopt the prior probability into the quantum state to form a Gram matrix, and employ the generalized $\alpha$-$z$-relative Rényi entropy of coherence of the Gram matrix to quantify the quantumness of the corresponding pure-state ensemble. In Section 2, we review the generalized $\alpha$-$z$-relative Rényi entropy and the related coherence measure, and the Gram matrix of a pure-state ensemble and its basic properties. Then we provide the quantifier of the quantumness of ensemble via coherence of the associated Gram matrix in terms of the generalized $\alpha$-$z$-relative Rényi entropy. We calculate this quantumness measure for six important ensembles and compare with several other quantifiers of quantumness. We conclude with a summary and some discussions in Section 3.

2 Quantumness of a Pure-State Ensemble via Generalized $\alpha$-$z$-Relative Rényi Entropy of Coherence

Let $\mathcal{H}$ be a $d$-dimensional Hilbert space, and $B\subset\mathcal{H}\Rightarrow$, $S\subset\mathcal{H}\Rightarrow$ and $D\subset\mathcal{H}\Rightarrow$ the set of all bounded linear operators, Hermitian operators and density operators on $\mathcal{H}$ (positive operators with trace 1), respectively. Let $\{ |i\rangle \}_{i=1}^{d}$ be an orthonormal basis of $\mathcal{H}$. A state is called incoherent if the density matrix is diagonal with respect to this basis. Denote by $\mathcal{I}$ the set of all incoherent states, $\mathcal{I} = \{ \delta \in D\subset\mathcal{H}\Rightarrow| \delta = \sum p_i |i\rangle\langle i|, p_i \geq 0, \sum p_i = 1 \}$. Let $\Phi$ be a completely positive trace preserving (CPTP) map, $\Phi(\rho) = \sum_i K_i \rho K_i^\dagger$, where $K_i$ are Kraus operators satisfying $\sum_i K_i^\dagger K_i = I_d$ with $I_d$ the identity operator. $K_i$ are called incoherent if $K_i^\dagger TK_i \in \mathcal{I}$ for all $i$, and the map is called incoherent. A well-defined coherence measure $C$ should satisfy the following conditions [33]: (C$_1$) (Faithfulness) $C(\rho) \geq 0$ and $C(\rho) = 0$ iff $\rho$ is incoherent. (C$_2$) (Monotonicity) $C(\Phi(\rho)) \leq C(\rho)$ for any incoherent operation $\Phi$. (C$_3$) (Convexity) $C(\cdot)$ is a convex function of $\rho$, i.e., $\sum p_i C(\rho_i) \geq C(\sum p_i \rho_i)$, where $p_i \geq 0$ and $\sum p_i = 1$. (C$_4$) (Strong monotonicity) $C(\cdot)$ does not increase on average under selective incoherent operations, i.e., $C(\rho) \geq \sum \rho_i C(\rho_i)$, where $\rho_i = \text{Tr}(K_i \rho K_i^\dagger)$ are probabilities and $K_i$ are post-measurement states, $K_i$ are incoherent Kraus operators. The conditions (C$_3$) and (C$_4$) can be replaced equivalently by the following additivity coherence for block-diagonal states [34], $C(pp_1 \oplus (1-p)p_2) = pC(p_1) + (1-p)C(p_2)$.

Also, denote the support of an operator $\rho$ by $\text{supp} \rho$. The support of an operator is defined to be the vector space orthogonal to its kernel. For a Hermitian operator, this means the vector space spanned by eigenvectors of the operator with non-zero eigenvalues. For any two quantum states $\rho, \sigma \in D\subset\mathcal{H}\Rightarrow$ with $\text{supp} \rho \subset \text{supp} \sigma$, the generalized $\alpha$-$z$-relative Rényi entropy is defined by [39],

$$D_{\alpha, z}(\rho, \sigma) = \frac{1}{\alpha - 1} (z^\alpha C(\rho, \sigma) - 1), \quad \alpha \in (-\infty, 1) \cup (1, +\infty), \quad z > 0,$$

where [35, 36, 39].

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\[ f_{a,\gamma}(\rho, \sigma) = \text{Tr}(\sigma^{i-\gamma} \rho^{\sigma^{i-\gamma}}). \]

Also, negative powers are defined in the sense of generalized inverses; that is, for negative \(x\), \(\rho^{-1} := (\rho^{\text{supp}})^{-1}\). For states \(\rho\) and \(\sigma\), (1) if \(0 < \alpha < 1\) and \(z > 0\), we have \(f_{a,\gamma}(\rho, \sigma) \leq 1\); (2) if \(\alpha > 1\) and \(z > 0\), we have \(f_{a,\gamma}(\rho, \sigma) \geq 1\). It is shown that when \(\alpha \to 1\) and \(z = 1\), \(D_{a,\gamma}(\rho, \sigma)\) reduces to \(S'(\rho|\sigma) = \text{Tr} \ln \rho - \text{Tr} \rho \ln \sigma\), where ‘\(\ln\)’ indicates a natural logarithm. Note that \(S'(\rho|\sigma) = \ln 2 \cdot S(\rho||\sigma)\) is the standard relative entropy between two quantum states \(\rho\) and \(\sigma\), in which the logarithm ‘\(\log\)’ is taken to base 2 \([37, 38]\).

The quantum coherence \(C_{a,\gamma}(\rho)\) of a state \(\rho\) is defined by \([39]\),
\[ C_{a,\gamma}(\rho) = \min_{\sigma \in \mathcal{I}} D_{a,\gamma}(\rho, \sigma), \tag{2} \]
which is a well-defined measure of coherence in the following cases \([39]\): (i) \(\alpha \in (0, 1)\) and \(z \geq \max\{\alpha, 1 - \alpha\}\); (ii) \(\alpha \in (1, 2]\) and \(z = 1\); (iii) \(\alpha \in (1, 2]\) and \(z = \frac{1}{\alpha}\); (iv) \(\alpha > 1\) and \(z = \alpha\). In particular, for \(\alpha \in (0, 1) \cup (1, 2]\) and \(z = 1\), the generalized \(a-z\)-relative Rényi entropy of coherence can be written as \([39]\),
\[ C_{a,1}(\rho) = \frac{\sum_{i=1}^{d} (\langle i|\rho^a|i \rangle)^{\frac{1}{z}} - 1}{\alpha - 1}. \tag{3} \]
In a similar manner, when \(\alpha \to 1\), \(C_{a,1}(\rho)\) reduces to \(\ln 2 \cdot C_{rel}(\rho)\), where \(C_{rel}(\rho)\) denotes the relative entropy of coherence defined in \([33]\).

Instead of a set \(\mathcal{S} = \{\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_n\rangle\}\) of \(n\) pure states in \(\mathcal{H}\), we consider a pure-state ensemble, \(\mathcal{E} = \{(p_i, |\psi_i\rangle) : i = 1, 2, \ldots, n\}\), where \(p_i > 0\) and \(\sum_i p_i = 1\). With respect to the set of vectors \(\{\sqrt{p_1}|\psi_1\rangle, \sqrt{p_2}|\psi_2\rangle, \ldots, \sqrt{p_n}|\psi_n\rangle\}\), the Gram matrix of \(\mathcal{E}\) is defined as \([32]\),
\[ G_\mathcal{E} = (\sqrt{p_i}|\psi_i\rangle\langle\psi_i|), \tag{4} \]
which is an \(n \times n\) matrix with elements \(\sqrt{p_i}|\psi_i\rangle\langle\psi_i|\). It is easy to see that the diagonal elements of \(G_\mathcal{E}\) are \(p_i\). It has been proved by Sun et al. \([32]\) that the Gram matrix of a pure-state ensemble (4) has the following properties.

(a) (State interpretation) \(G_\mathcal{E}\) is a non-negative semidefinite matrix satisfying \(\text{Tr} G_\mathcal{E} = 1\). \(G_\mathcal{E}\) is diagonal if and only if the pure states in the ensemble \(\mathcal{E}\) are mutually orthogonal.
(b) (Unitary invariance) \(G_{U_\mathcal{E}} = G_\mathcal{E}\) for any unitary operator \(U\) on \(\mathcal{H}\), where \(U\mathcal{E} = \{(p_i, U|\psi_i\rangle) : i = 1, 2, \ldots, n\}\).
(c) (Hadamard multiplicability) Denote \(\mathcal{E}_1 \circ \mathcal{E}_2 = \{(p_i q_i, |\psi_i\rangle \otimes |\phi_i\rangle) : i = 1, 2, \ldots, n\}\) for two ordered quantum ensembles \(\mathcal{E}_1 = \{(p_i, |\psi_i\rangle) : i = 1, 2, \ldots, n\}\) and \(\mathcal{E}_2 = \{(q_i, |\phi_i\rangle) : i = 1, 2, \ldots, n\}\). Then \(G_{\mathcal{E}_1 \circ \mathcal{E}_2} = G_{\mathcal{E}_1} \otimes G_{\mathcal{E}_2}\) where \(A \otimes B = (a_{ij}) B = (b_{ij})\) denotes the matrix Hadamard product of \(n \times n\) matrices \(A = (a_{ij})\) and \(B = (b_{ij})\).
(d) (Tensor multiplicability) For any two quantum ensembles \(\mathcal{E} = \{(p_i, |\psi_i\rangle) : i = 1, 2, \ldots, n\}\) and \(\mathcal{F} = \{(q_k, |\phi_k\rangle) : k = 1, 2, \ldots, m\}\), denote \(\mathcal{E} \otimes \mathcal{F} = \{(p_i q_k, |\psi_i\rangle \otimes |\phi_k\rangle) : i = 1, 2, \ldots, n, k = 1, 2, \ldots, m\}\). Then \(G_{\mathcal{E} \otimes \mathcal{F}} = G_\mathcal{E} \otimes G_\mathcal{F}\).

The cross Gram matrix between \(\mathcal{E}\) and \(\mathcal{F}\) is defined by \([32]\), \(G_{\mathcal{E} \otimes \mathcal{F}} = (\sqrt{p_i q_k} |\psi_i\rangle \langle\psi_i| \phi_k\rangle)\). It has been proved that \([32]\) \(G_{U_\mathcal{E} U_\mathcal{F}} = G_{\mathcal{E}, \mathcal{F}}\) for any unitary operator \(U\) on \(\mathcal{H}\). When \(\mathcal{E} = \mathcal{F}\), one has \(G_{\mathcal{E}, \mathcal{E}} = G_\mathcal{E}\).
From the property (a), we can view $G_{\mathcal{E}}$ as a density matrix in an $n$-dimensional Hilbert space. Let $\mathcal{E} = \{(p_i, |\psi_i\rangle) : i = 1, 2, \ldots, n\}$ be a pure-state ensemble, and $G_{\mathcal{E}} = (\sqrt{p_i} \langle \psi_i | \psi_j \rangle)$ the corresponding Gram matrix. We define the quantumness of a pure-state ensemble $\mathcal{E}$ as the coherence of the Gram matrix $G_{\mathcal{E}}$ based on the generalized $\alpha$-z-relative Rényi entropy,

$$Q_{\alpha, z}(\mathcal{E}) = C_{\alpha, z}(G_{\mathcal{E}}).$$

(5)

By (1) and (2), (5) can be rewritten as,

$$Q_{\alpha, z}(\mathcal{E}) = \min_{\sigma \in \mathcal{L}} \frac{1}{\alpha - 1} \log \frac{f_{\alpha, z}(G_{\mathcal{E}}, \sigma)}{d_{\alpha, z}(G_{\mathcal{E}})}.$$

(6)

For any $\alpha, z$ satisfying one of the cases (i)-(iv) below Eq. (2), the quantumness measure $Q_{\alpha, z}(\cdot)$ has the following desirable properties.

1. **(Positivity)** $Q_{\alpha, z}(\mathcal{E}) \geq 0$ with equality holding if and only if $\mathcal{E}$ is a classical ensemble in the sense that the pure states in the ensemble are mutually orthogonal. This is due to that $C_{\alpha, z}(\cdot)$ is a well-defined coherence measure, namely, $C_{\alpha, z}(\mathcal{E}) \geq 0$, which implies that $Q_{\alpha, z}(\mathcal{E}) \geq 0$. Moreover, $Q_{\alpha, z}(\mathcal{E}) = 0$ iff $C_{\alpha, z}(G_{\mathcal{E}}) = 0$ iff $G_{\mathcal{E}}$ is diagonal iff the pure states in the ensemble are pairwise orthogonal.

2. **(Unitary invariance)** $Q_{\alpha, z}(\cdot)$ is unitary invariant in the sense that $Q_{\alpha, z}(U\mathcal{E}) = Q_{\alpha, z}(\mathcal{E})$ for any unitary operator $U$ on $\mathcal{H}$, where $U\mathcal{E} = \{(p_i, U|\psi_i\rangle) : i = 1, 2, \ldots, n\}$. This can be seen from the properties of the cross Gram matrix between two pure-state ensembles. For any unitary operator $U$ on $\mathcal{H}$, it holds that $G_{U\mathcal{E}} = G_{\mathcal{E}, U\mathcal{E}} = G_{\mathcal{E}, \mathcal{E}} = G_{\mathcal{E}}$, which gives rise to $Q_{\alpha, z}(U\mathcal{E}) = Q_{\alpha, z}(\mathcal{E})$.

3. **(Subadditivity)** $Q_{\alpha, z}(\cdot)$ is subadditive after normalization in the sense that

$$Q'_{\alpha, z}(\mathcal{E} \otimes \mathcal{F}) \leq Q'_{\alpha, z}(\mathcal{E}) + Q'_{\alpha, z}(\mathcal{F}),$$

(7)

for any two quantum ensembles $\mathcal{E} = \{(p_i, |\psi_i\rangle) : i = 1, 2, \ldots, n\}$ and $\mathcal{F} = \{(q_k, |\phi_k\rangle) : k = 1, 2, \ldots, m\}$. Here $Q'_{\alpha, z}(\mathcal{E}) = Q_{\alpha, z}(\mathcal{E})/n$ and $Q'_{\alpha, z}(\mathcal{F}) = Q_{\alpha, z}(\mathcal{F})/m$ with $n$ and $m$ being the number of quantum states in the ensembles $\mathcal{E}$ and $\mathcal{F}$, respectively, and the tensor product of two quantum ensembles is defined as $\mathcal{E} \otimes \mathcal{F} = \{(p_i q_k, |\psi_i\rangle \otimes |\phi_k\rangle) : i = 1, 2, \ldots, n, k = 1, 2, \ldots, m\}$. The proof of property (3) is given in the appendix.

We calculate the quantumness defined by (5) for several important ensembles and compare them with other quantifiers of quantumness proposed in previous literatures.

**Example 1** Consider the B92 ensemble on $\mathbb{C}^2$ [40],

$$\mathcal{E}_x = \left\{ \left( \frac{1}{2}, |\psi_1\rangle \right), \left( \frac{1}{2}, |\psi_2\rangle \right) \right\},$$

where $\langle \psi_1 | \psi_2 \rangle = \sin \theta = x$, $\theta \in [0, \frac{\pi}{2}]$, and $|\psi_1\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} |1\rangle$, $|\psi_2\rangle = \sin \frac{\theta}{2} |0\rangle + \cos \frac{\theta}{2} |1\rangle$. The Gram matrix of $\mathcal{E}_x$ is

$$G_{\mathcal{E}_x} = \frac{1}{2} \begin{pmatrix} 1 & x \\ x & 1 \end{pmatrix}$$

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with eigenvalues $\frac{1}{2} \pm x$. By direct computation we have the quantumness of $E_x$, 
\[
Q_{a,1}(E_x) = \frac{2^{\frac{1}{\alpha}}[(1-x)^{\alpha} + (1+x)^{\alpha}]^\frac{1}{\alpha} - 1}{\alpha - 1},
\]
which captures the overlap between $|\psi_1\rangle$ and $|\psi_2\rangle$. In particular, when $x = \frac{1}{\sqrt{2}}$, we have 
\[
Q_{a,1}(E_{B92}) = \frac{2^{\frac{1}{\alpha}}[(1 - \frac{1}{\sqrt{2}})^{\alpha} + (1 + \frac{1}{\sqrt{2}})^{\alpha}]^\frac{1}{\alpha} - 1}{\alpha - 1},
\]
where $E_{B92} = E_{\frac{1}{\sqrt{2}}}$, and $\lim_{\alpha \to 1} Q_{a,1}(E_{B92}) \approx 0.28$.

**Example 2** Consider the diagonal ensemble [22], 
\[
E_{\text{diag}} = \left\{ \left( \frac{1}{3}, |0\rangle \right), \left( \frac{1}{3}, |1\rangle \right), \left( \frac{1}{3}, |+\rangle \right) \right\},
\]
where $|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$. The Gram matrix of $E_{\text{diag}}$ is 
\[
G_{E_{\text{diag}}} = \frac{1}{3} \begin{pmatrix}
1 & 0 & \frac{1}{\sqrt{2}} \\
0 & 1 & \frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 1
\end{pmatrix}
\]
with eigenvalues $\frac{2}{3}, \frac{1}{3}, 0$. Direct computation shows that the quantumness of $E_{\text{diag}}$ is 
\[
Q_{a,1}(E_{\text{diag}}) = \frac{2^{\frac{1}{\alpha}} [(1 + 2^{a - 1})^\frac{1}{\alpha} + 1] - 3}{3(\alpha - 1)},
\]
and $\lim_{\alpha \to 1} Q_{a,1}(E_{\text{diag}}) \approx 0.46$.

**Example 3** Consider the trine ensemble [41–46], 
\[
E_{\text{trine}} = \left\{ \left( \frac{1}{3}, |0\rangle \right), \left( \frac{1}{3}, \frac{1}{2} |0\rangle + \frac{\sqrt{3}}{2} |1\rangle \right), \left( \frac{1}{3}, \frac{1}{2} |0\rangle - \frac{\sqrt{3}}{2} |1\rangle \right) \right\}.
\]
The Gram matrix of $E_{\text{trine}}$ is 
\[
G_{E_{\text{trine}}} = \frac{1}{6} \begin{pmatrix}
2 & 1 & 1 \\
1 & 2 & -1 \\
1 & -1 & 2
\end{pmatrix}
\]
with eigenvalues $\frac{1}{2}, \frac{1}{2}, 0$. Direct computation shows that the quantumness of $E_{\text{trine}}$ is 
\[
Q_{a,1}(E_{\text{trine}}) = \frac{(\frac{2}{3})^{\frac{1}{\alpha}} - 1}{\alpha - 1},
\]
and $\lim_{\alpha \to 1} Q_{a,1}(E_{\text{trine}}) \approx 0.41$.

**Example 4** Consider the BB84 ensemble [47],
\[ \mathcal{E}_{BB84} = \left\{ \left( \frac{1}{4}, |0\rangle \right), \left( \frac{1}{4}, |1\rangle \right), \left( \frac{1}{4}, |+\rangle \right), \left( \frac{1}{4}, |\rangle \right) \right\}, \]

where \(|\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}}\). The Gram matrix of \(\mathcal{E}_{BB84}\) is

\[
G_{\mathcal{E}_{BB84}} = \frac{1}{4\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 1 & 1 \\ 0 & \sqrt{2} & 1 & -1 \\ 1 & 1 & \sqrt{2} & 0 \\ 1 & -1 & 0 & \sqrt{2} \end{pmatrix}
\]

with eigenvalues \(\frac{1}{2}, \frac{1}{2}, 0, 0\). Direct computation shows that the quantumness of \(\mathcal{E}_{BB84}\) is

\[
Q_{\alpha,1}(\mathcal{E}_{BB84}) = \frac{2^{\frac{1}{\alpha}}}{\alpha - 1},
\]

and \(\lim_{\alpha \to 1} Q_{\alpha,1}(\mathcal{E}_{BB84}) \approx 0.69\).

**Example 5** Consider the tetrad ensemble [46],

\[ \mathcal{E}_{tetrad} = \{(p_j, |\psi_j\rangle) : j = 1, 2, 3, 4\} \]

with \(p_j = \frac{1}{4}\) \((j = 1, 2, 3, 4)\), and

\[
|\psi_1\rangle = |0\rangle, \quad |\psi_2\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle, \quad |\psi_3\rangle = \frac{1}{\sqrt{3}}|0\rangle + e^{\frac{2\pi i}{3}}\sqrt{\frac{2}{3}}|1\rangle, \quad |\psi_4\rangle = \frac{1}{\sqrt{3}}|0\rangle + e^{\frac{4\pi i}{3}}\sqrt{\frac{2}{3}}|1\rangle.
\]

A symmetric informationally complete (SIC) set in a Hilbert space \(\mathcal{H}\) with dimension \(d\) [48, 49] is a set of \(d^2\) pure states \(|\psi_j\rangle\) such that

\[
|\langle \psi_j | \psi_k \rangle|^2 = \frac{1}{d + 1}, \quad j \neq k.
\]

It is easy to see that \(\{|\psi_j\rangle : j = 1, 2, 3, 4\}\) in \(\mathcal{E}_{tetrad}\) is a SIC set in \(\mathbb{C}^2\). The Gram matrix of the ensemble \(\mathcal{E}_{tetrad}\) is

\[
G_{\mathcal{E}_{tetrad}} = \frac{1}{4\sqrt{3}} \begin{pmatrix} \sqrt{3} & 1 & 1 & 1 \\ 1 & \sqrt{3} & i & -i \\ 1 & -i & \sqrt{3} & i \\ 1 & i & -i & \sqrt{3} \end{pmatrix}
\]

with eigenvalues \(\frac{1}{2}, \frac{1}{2}, 0, 0\). Direct computation shows that the quantumness of \(\mathcal{E}_{tetrad}\) is

\[
Q_{\alpha,1}(\mathcal{E}_{tetrad}) = \frac{2^{\frac{1}{\alpha}}}{\alpha - 1},
\]

and \(\lim_{\alpha \to 1} Q_{\alpha,1}(\mathcal{E}_{tetrad}) \approx 0.69\).
**Example 6** Consider the six-state ensemble [49–53]

\[ \mathcal{E}_{\text{six}} = \left\{ \left( \frac{1}{6}, |0_\mu\rangle \right), \left( \frac{1}{6}, |1_\mu\rangle \right) : \mu = x, y, z \right\} \]

on \( \mathbb{C}^2 \), where \(|0_z\rangle = |0\rangle, |1_z\rangle = |1\rangle\), and

\[ |0_z\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}, \quad |1_z\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}. \]

\[ |0_y\rangle = \frac{|0\rangle + i|1\rangle}{\sqrt{2}}, \quad |1_y\rangle = \frac{|0\rangle - i|1\rangle}{\sqrt{2}}. \]

The Gram matrix of the ensemble \( \mathcal{E}_{\text{six}} \) is

\[
G_{\mathcal{E}_{\text{six}}} = \frac{1}{12} \begin{pmatrix}
2 & 0 & 1 + i & 1 - i & \sqrt{2} & \sqrt{2} \\
0 & 2 & 1 - i & 1 + i & -\sqrt{2} & \sqrt{2} \\
1 - i & 1 + i & 0 & 2 & \sqrt{2} & -\sqrt{2} \\
1 + i & 1 - i & 0 & 2 & -\sqrt{2} & \sqrt{2} \\
\sqrt{2} & \sqrt{2} & \sqrt{2} & \sqrt{2} & 2 & 2 \\
\sqrt{2} & \sqrt{2} & \sqrt{2} & \sqrt{2} & 2 & 0 \\
\end{pmatrix}
\]

with eigenvalues \( \frac{1}{2}, \frac{1}{2}, 0, 0, 0, 0 \). Direct computation shows that the quantumness of \( \mathcal{E}_{\text{six}} \) is

\[
Q_{\alpha,1}(\mathcal{E}_{\text{six}}) = \frac{3^\frac{\alpha-1}{\alpha} - 1}{\alpha - 1}, \tag{14}
\]

and \( \lim_{\alpha \to 1} Q_{\alpha,1}(\mathcal{E}_{\text{six}}) \approx 1.10 \). The values of \( \lim_{\alpha \to 1} Q_{\alpha,1}(\cdot) \) for the six pure-state ensembles in the above examples differ from the ones \( Q_{\alpha,1}(\cdot) \) in Table 1 of Ref. [32] by a constant factor \( \ln 2 \).

Note that the BB84 ensemble, the six-state ensemble and so on are all treated as complete mixed state, or classical state in other words, if viewed from the entanglement. However, they look differently from the quantumness defined via the generalized \( \alpha \)-\( z \)-relative Rényi entropy of coherence.

It follows from (12) and (13) that \( Q_{\alpha,1}(\mathcal{E}_{\text{BB84}}) = Q_{\alpha,1}(\mathcal{E}_{\text{tetrad}}) \). In addition, by (9) and (11), \( Q_{2,1}(\mathcal{E}_{\text{BB84}}) = Q_{2,1}(\mathcal{E}_{\text{trine}}) = \sqrt{\frac{3}{2}} - 1 \). We have the following observations, see Fig. 1.

**Fig. 1** The quantumness \( Q_{\alpha,1}(\cdot) \) of ensembles

![Q_\alpha_1 vs \alpha for different ensembles](image-url)
Among the six ensembles, \( Q_{a,1}(E_{B92}) \) is always the minimum, while \( Q_{a,1}(E_{six}) \) is always the maximum for all \( \alpha \). For any fixed \( \alpha \), one has the following ordering,

\[
Q_{a,1}(E_{B92}) \leq Q_{a,1}(E_{trine}) \leq Q_{a,1}(E_{BB84}) = Q_{a,1}(E_{tetrad}) \leq Q_{a,1}(E_{six})
\]

and

\[
Q_{a,1}(E_{B92}) \leq Q_{a,1}(E_{diag}) \leq Q_{a,1}(E_{BB84}) = Q_{a,1}(E_{tetrad}) \leq Q_{a,1}(E_{six}).
\]

The curves of \( Q_{a,1}(E_{BB84}) \) and \( Q_{a,1}(E_{tetrad}) \) coincides as \( Q_{a,1}(E_{BB84}) = Q_{a,1}(E_{tetrad}) \). There is no ordering between \( Q_{a,1}(E_{trine}) \) and \( Q_{a,1}(E_{diag}) \) for \( \alpha \in (0,1) \cup (1,2] \) in general. In fact, \( Q_{a,1}(E_{trine}) = Q_{a,1}(E_{diag}) \) when \( \alpha = \alpha_c \approx 0.33 \), and we have \( Q_{a,1}(E_{trine}) \geq Q_{a,1}(E_{diag}) \) when \( \alpha \in (0,\alpha_c) \), while \( Q_{a,1}(E_{trine}) \leq Q_{a,1}(E_{diag}) \) when \( \alpha \in (\alpha_c,1) \cup (1,2] \).

In order to get a more intuitive picture of the quantumness of quantum ensembles, we next compare our quantifiers with some existing ones in the literatures. For a ensemble \( \mathcal{E} = \{(p_i, |\psi_i\rangle) : i = 1, 2, \ldots, n\} \) on a Hilbert space \( \mathcal{H} \), the quantumness based on the \( l_1 \)-norm of coherence of the Gram matrix is defined by [33, 54–56],

\[
Q_{l_1}(\mathcal{E}) = \sum_{i \neq j} \sqrt{p_i p_j} |\langle \psi_i | \psi_j \rangle|.
\]

The quantumness based on the security of information transmission is defined by [20–23],

\[
Q_{FS}(\mathcal{E}) = 1 - \sup_{M, \{\sigma_k\}} \sum_{i,k} p_i \text{Tr}(|\psi_i\rangle\langle \psi_i| M_k) \text{Tr}(|\psi_i\rangle\langle \psi_i| \sigma_k),
\]

where the sup carries out with respect to all measurements \( M = \{M_k\} \) on \( \mathcal{H} \) and sets of quantum states \( \{\sigma_k\} \). In [22] the quantumness based on quantum cloning is defined to be,

\[
Q_{clon}(\mathcal{E}) = 1 - \sup_{U} \sum_{i} p_i |\langle \psi_i | \otimes \langle \psi_i| U |\psi_i \rangle \otimes |0\rangle|^2,
\]

where the sup goes over all unitary operators \( U \) on the composite system \( \mathcal{H} \otimes \mathcal{H} \) such that \( U(|\psi_i\rangle \otimes |0\rangle) = |\psi_i\rangle \) has the same marginals, and \( |0\rangle \in \mathcal{H} \) is any fixed pure state. Instead of \( Q_{clon}(\mathcal{E}) \), a modified version \( Q'_{clon}(\mathcal{E}) \) is also considered by implementing a symmetric unitary operator when optimizing over \( U \), which is easier to calculate. The quantumness based on the Holevo quantity and the accessible information is given by [22, 45],

\[
Q_{Hol}(\mathcal{E}) = \chi(\mathcal{E}) - \chi_0(\mathcal{E}),
\]

where

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
 & \( E_{B92} \) & \( E_{diag} \) & \( E_{trine} \) & \( E_{BB84} \) & \( E_{tetrad} \) & \( E_{six} \) \\
\hline
\( Q_{a,1} \) & (9) & (10) & (11) & (12) & (13) & (14) \\
\( Q_{I} \) & 0.71 & 0.94 & 1 & 1.41 & 1.73 & 2.83 \\
\( Q_{FS} \) & 0.07 & 0.13 & 0.25 & 0.25 & 0.33 & 0.33 \\
\( Q_{clon} \) & 0.02 & 0.10 & 0.32 & 0.32 & 0.34 & 0.35 \\
\( Q_{Hol} \) & 0.20 & 0.25 & 0.42 & 0.50 & 0.59 & 0.67 \\
\( Q_{comm} \) & 0.25 & 0.22 & 0.25 & 0.25 & 0.33 & 0.33 \\
\( Q \) & 0.50 & 0.67 & 0.75 & 1 & 1.33 & 2 \\
\hline
\end{tabular}
\caption{Comparison of different quantifiers of quantumness of pure-state ensembles}
\end{table}
\[
\chi(\mathcal{E}) = S\left(\sum_i p_i |\psi_i\rangle\langle \psi_i|\right) - \sum_i p_i S(|\psi_i\rangle\langle \psi_i|)
\]

is the Holevo quantity of the pure-state ensemble \(\mathcal{E} = \{(p_i, |\psi_i\rangle) : i = 1, 2, \cdots, n\}\), while \(\chi_0(\mathcal{E}) = \sup_M I(M(\mathcal{E}))\) is the accessible information, in which the sup is conducted over all measurements \(M = \{M_k\}\) on \(\mathcal{H}\), and

\[
I(M(\mathcal{E})) = -\sum_i p_i \log p_i - \sum_k q_k \log q_k + \sum_{ik} q_{ik} \log q_{ik}
\]

denotes the mutual information of the joint probability distribution \(q_{ik} = p_i \text{Tr}(|\psi_i\rangle\langle \psi_i| M_k)\) with marginals \(\{p_i = \sum_k q_{ik}\}\) and \(\{q_k = \sum_i q_{ik}\}\). The quantumness based on the commutator is defined by [27–29],

\[
Q(\mathcal{E}) = -\sum_{ij} \sqrt{p_ip_j} \text{Tr}[|\psi_i\rangle\langle \psi_i|, |\psi_j\rangle\langle \psi_j|] \times 2,
\]

and

\[
Q_{\text{comm}}(\mathcal{E}) = -\sum_{ij} p_ip_j \text{Tr}[|\psi_i\rangle\langle \psi_i|, |\psi_j\rangle\langle \psi_j|] \times 2.
\]

Combining (9)-(14), the Table 2 in [32] and the results in [22], we have the Table 1, which gives a comparison among the different quantifiers of quantumness for these pure-state ensembles.

In Fig. 2 we plot the quantumness of the six ensembles based on different quantifiers. We have the following observations:

1. For \(Q_{\text{comm}}(\cdot)\), the quantumness of the ensemble \(\mathcal{E}_{\text{diag}}\) is the minimum, while the quantumness of ensemble \(\mathcal{E}_{\text{six}}\) is the maximum. In comparison, for other quantifiers, the quantumness of \(\mathcal{E}_{\text{B92}}\) is the minimum, while the quantumness of \(\mathcal{E}_{\text{six}}\) remains the maximum. For any fixed \(\alpha\), \(Q_{\text{comm}}(\cdot)\) yields the following ordering for quantumness of ensembles,

\[
\mathcal{E}_{\text{diag}} \leq \mathcal{E}_{\text{B92}} \leq \mathcal{E}_{\text{trine}} \leq \mathcal{E}_{\text{BB84}} \leq \mathcal{E}_{\text{tetrad}} \leq \mathcal{E}_{\text{six}},
\]

while other quantifiers yield consistent orderings for quantumness of ensembles,

\[
\mathcal{E}_{\text{B92}} \leq \mathcal{E}_{\text{diag}} \leq \mathcal{E}_{\text{BB84}} \leq \mathcal{E}_{\text{tetrad}} \leq \mathcal{E}_{\text{six}}
\]

and

\[
\mathcal{E}_{\text{B92}} \leq \mathcal{E}_{\text{trine}} \leq \mathcal{E}_{\text{BB84}} \leq \mathcal{E}_{\text{tetrad}} \leq \mathcal{E}_{\text{six}}.
\]

2. Some quantifiers yield strict orderings for the considered ensembles mentioned in observation (1), while other ones yield the same values for two or three ensembles, as pointed out in Ref. [32].

3. For a given ensemble among the considered ones, it is shown that \(Q_{\alpha,1}(\cdot)\) coincides with the quantumness based on one or more quantifiers for different \(\alpha\).

- For the B92 ensemble, the quantumness \(Q_{\alpha,1}(\mathcal{E}_{\text{B92}}) = Q_{\text{comm}}(\mathcal{E}_{\text{B92}})\) when \(\alpha \approx 1.53\).
• For the diagonal ensemble, the quantumness $Q_{a,1}(E_{\text{diag}}) = Q_{l}(E_{\text{diag}})$ when $\alpha \approx 0.23$; the quantumness $Q_{a,1}(E_{\text{diag}}) = Q(E_{\text{diag}})$ when $\alpha \approx 0.54$.
• For the trine ensemble, the quantumness $Q_{a,1}(E_{\text{trine}}) = Q_{l}(E_{\text{trine}})$ when $\alpha \approx 0.20$; the quantumness $Q_{a,1}(E_{\text{trine}}) = Q_{\text{FS}}(E_{\text{trine}})$ and $Q_{a,1}(E_{\text{trine}}) = Q_{\text{comm}}(E_{\text{trine}})$ when $\alpha \approx 1.77$.

Fig. 2 The quantumness of ensembles based on different quantifiers for a pure-state ensemble: (a) the B92 ensemble $E_{\text{B92}}$; (b) the diagonal ensemble $E_{\text{diag}}$; (c) the trine ensemble $E_{\text{trine}}$; (d) the BB84 ensemble $E_{\text{BB84}}$; (e) the tetrad ensemble $E_{\text{tetrad}}$; (f) the six-state ensemble $E_{\text{six}}$. The $Q$-axis denotes the quantumness with respect to various quantifiers.
the quantumness $Q_{a,1}(\mathcal{E}_{\text{trine}}) = Q'_{\text{clon}}(\mathcal{E}_{\text{trine}})$ when $\alpha \approx 1.33$; the quantumness $Q_{a,1}(\mathcal{E}_{\text{trine}}) = Q_{\text{Hol}}(\mathcal{E}_{\text{trine}})$ when $\alpha \approx 0.96$; the quantumness $Q_{a,1}(\mathcal{E}_{\text{trine}}) = Q(\mathcal{E}_{\text{trine}})$ when $\alpha \approx 0.41$.

• For the BB84 ensemble, the quantumness $Q_{a,1}(\mathcal{E}_{\text{BB84}}) = Q_{\text{Hol}}(\mathcal{E}_{\text{BB84}})$ when $\alpha \approx 1.59$; the quantumness $Q_{a,1}(\mathcal{E}_{\text{BB84}}) = Q(\mathcal{E}_{\text{BB84}})$ when $\alpha = 0.50$.

• For the tetrad ensemble, the quantumness $Q_{a,1}(\mathcal{E}_{\text{tetrad}}) = Q_{\text{Hol}}(\mathcal{E}_{\text{tetrad}})$ when $\alpha \approx 1.26$.

3 Conclusions

Following the ideas in [32], we have employed the generalized $\alpha$-z-relative Rényi entropy of coherence of Gram matrix to quantify the quantumness of pure-state ensembles and explored its basic properties. Furthermore, we have calculated the newly-defined quantumness for six ensembles and presented the explicit formulas with parameter $\alpha$. These ensembles arise in quantum cryptography or quantum measurement. We have plotted the images of these quantumness measures as a function of $\alpha$. It is found that for fixed $\alpha$, $Q_{a,1}(\mathcal{E}_{\text{BB92}})$ is always the minimum, while $Q_{a,1}(\mathcal{E}_{\text{six}})$ is always the maximum. There is an order of the corresponding quantities. Moreover, we have also compared the quantumness of the six ensembles with other quantumness quantifiers. It can be seen that different quantifiers may yield different orderings of the quantumness for the six ensembles. By plotting the images of the quantumness based on various quantifiers for the same chosen pure-state ensemble respectively, we have observed that the curves of $Q_{a,1}(\cdot)$ intersects with the lines of other quantifiers at different $\alpha$. This fact highlights the complexity and subtlety of the quantumness measure since different quantifiers may capture different aspects of the ensemble.

Our result enforces the previous finding in Refs. [57, 58] that though the density matrix of two ensembles are identical, they differ in physics. In their work, they used the general fluctuations, to distinguish them. It may be a future topic to see if there is any link between the two quantities, the fluctuation, and our quantumness defined via the generalized $\alpha$-z-relative Rényi entropy of coherence.

The quantumness of pure-state ensembles defined in this paper may play a very important role in quantum information, such as quantum key distribution [47, 59], quantum secure direct communication [60, 61]. It is more capable than entanglement [62, 63] in that they can enable the secure transfer of information. It may also shed some light on understanding the nature of measurement in quantum mechanics [64, 65].

Since a general ensemble consists of mixed quantum states, it is necessary to extend our results from pure-state ensembles to the case of mixed state ensembles. This important issue deserves further study.

Appendix: Proof of the subadditivity of the quantumness $Q_{a,z}(\cdot)$

According to (6), we have

$$Q'_{a,z}(\mathcal{E} \otimes \mathcal{F}) = \min_{\sigma_1 \in \mathcal{I}_1, \sigma_2 \in \mathcal{I}_2} \frac{\int_{m(a-1)}^{1} (G_{\sigma_2, \sigma_1 \otimes \sigma_2})^{-1} \, dm - a}{mn(a-1)},$$

$$Q'_{a,z}(\mathcal{E}) = \min_{\sigma_1 \in \mathcal{I}_1} \frac{\int_{m(a-1)}^{1} (G_{\sigma_1})^{-1} \, dm - a}{mn(a-1)},$$

$$Q'_{a,z}(\mathcal{F}) = \min_{\sigma_2 \in \mathcal{I}_2} \frac{\int_{m(a-1)}^{1} (G_{\sigma_2})^{-1} \, dm - a}{mn(a-1)},$$

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where $I_1$ and $I_2$ denotes the set of incoherent states on the $m$-dimensional and $n$-dimensional Hilbert spaces, respectively. By the tensor multiplicability of the Gram matrix, i.e., $G_{E\otimes F} = G_E \otimes G_F$, we have

\[
\begin{align*}
    f_{a,z}^1(G_{E\otimes F}, \sigma_1 \otimes \sigma_2) &= \{ \text{Tr}[\sigma_1 \otimes \sigma_2] = G_{E\otimes F}^z(\sigma_1 \otimes \sigma_2) \}^\frac{1}{z} \\
    &= \{ \text{Tr}[\sigma_1] = G_{E}^z(\sigma_1) \}^\frac{1}{z} \cdot \{ \text{Tr}[\sigma_2] = G_{F}^z(\sigma_2) \}^\frac{1}{z} \\
    &= f_{a,z}^1(G_E, \sigma_1) \cdot f_{a,z}^1(G_F, \sigma_2).
\end{align*}
\]

So in order to prove the subadditivity, we only need to prove that

\[
\begin{align*}
\min_{\sigma_1 \in I_1, \sigma_2 \in I_2} f_{a,z}^1(G_E, \sigma_1) \cdot f_{a,z}^1(G_F, \sigma_2) &\leq \min_{\sigma_1 \in I_1} f_{a,z}^1(G_E, \sigma_1) - 1 + \min_{\sigma_2 \in I_2} f_{a,z}^1(G_F, \sigma_2) - 1. \\
\end{align*}
\]

Case (i): $0 < \alpha \leq 1, z > 0$. Since the matrix $\sigma^\frac{1}{z} = \rho^\frac{1}{z} \sigma^\frac{1}{z}$ has real, non-negative eigenvalues, we obtain $f_{a,z}^1(G_E, \sigma_1) \geq 0$ and $f_{a,z}^1(G_F, \sigma_2) \geq 0$. Noting that $f_{a,z}^1(\rho, \sigma) \leq 1$ when $0 < \alpha < 1$, we have $0 \leq f_{a,z}^1(G_E, \sigma_1) \leq 1$ and $0 \leq f_{a,z}^1(G_F, \sigma_2) \leq 1$, which implies that

\[
(f_{a,z}^1(G_E, \sigma_1) - n)(f_{a,z}^1(G_F, \sigma_2) - m) \geq (1 - n)(1 - m) \tag{16}
\]

for each $\sigma_1 \in I_1$ and $\sigma_2 \in I_2$. Hence, (15) holds.

Case (ii): $1 < \alpha \leq 2, z > 0$. Since the completely mixed state $\sigma = I/d$ is a diagonal matrix, which is an incoherent state, we have $\min_{\sigma \in I} f_{a,z}^1(\rho, \sigma) \leq f_{a,z}^1(\rho, \sigma) = (d^{a-1} \text{Tr}(\rho^a))^\frac{1}{z} \leq d$.

Noting that $f_{a,z}^1(\rho, \sigma) \geq 1$ when $\alpha > 1$, we have $1 \leq \min_{\sigma_1 \in I_1} f_{a,z}^1(G_E, \sigma_1) \leq n$ and $1 \leq \min_{\sigma_2 \in I_2} f_{a,z}^1(G_F, \sigma_2) \leq m$, which implies that

\[
\min_{\sigma_1 \in I_1} f_{a,z}^1(G_E, \sigma_1) \cdot \min_{\sigma_2 \in I_2} f_{a,z}^1(G_F, \sigma_2) - 1 \leq m \left( \min_{\sigma_1 \in I_1} f_{a,z}^1(G_E, \sigma_1) - 1 \right) + n \left( \min_{\sigma_2 \in I_2} f_{a,z}^1(G_F, \sigma_2) - 1 \right),
\]

and thus (15) holds.

In either case, we have proved (15), and so (7) is established. This completes the proof.

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Declarations

Competing interests The authors declare no competing interests.

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