Maximum coherence in the optimal basis

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The resource theoretic measure of quantum coherence is basis dependent, and the amount of coherence contained in a state is different in different bases. We obtained analytical solutions for the maximum coherence by optimizing the reference basis and highlighted the essential role of the mutually unbiased bases (MUBs) on attaining the maximum coherence. Apart from the relative entropy of coherence, we showed that the MUBs are optimal for the robustness of coherence, the coherence weight, and the modified skew information measure of coherence for any state. Moreover, the MUBs are optimal for all the faithful coherence measures if the state is pure or is of the single qubit. We also highlighted an upper bound for the $l_1$ norm of coherence and compared it with the other bounds as well as the maximum one attainable by optimizing the reference basis.

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I. INTRODUCTION

Quantum coherence is a basic feature of quantum states that is more fundamental than the other quantum features such as Bell nonlocality, entanglement, and quantum discord [1,2]. It also plays an essential role in the study of the reference frames [3–5], quantum thermodynamics [6–10], and biological systems [11, 12]. Meanwhile, coherence was recognized to be a precious resource for various quantum information processing tasks that cannot be accomplished in a classical way [13–17]. Despite these importance, a physically meaningful and mathematically rigorous framework for quantifying coherence was formulated only recently [18]. In this framework, the coherence measures were defined in the similar vein to those of the quantum correlation measures [1], with the free states, the free operations, and the unit resource states being identified explicitly as the incoherent states, the incoherent operations (I Os), and the maximally coherent states, respectively [18].

Based on the above framework, there are various coherence measures being proposed until now. Besides the relative entropy of coherence and $l_1$ norm of coherence [18], other faithful measures include the entanglement-based coherence measure [19], the robustness of coherence (RoC) [13, 14] and the coherence weight [20], the modified skew information measure of coherence [21], the two convex roof measures of coherence which are called intrinsic randomness of coherence [22] (also known as the coherence of formation [23]) and coherence concurrence [24], the discord-like bipartite coherence [25], and an operational coherence measure defined based on the max-relative entropy [26]. Moreover, there are other measures that obey partial of the conditions suggested in Ref. [18], e.g., the skew information measure of coherence, which is also a well-defined measure of asymmetry [27], the Tsallis relative entropy measure of coherence [28], and the trace norm of coherence [29, 50]. By identifying the free operations to be the genuinely incoherent operations which give $\Phi_{\text{GIO}}(\delta) = \delta$ for all the incoherent states $\delta \in \mathcal{I}$, the genuine quantum coherence was also introduced recently [31].

As the coherence measures are basis dependent, it is natural to wonder in which basis a state attains its maximum amount of coherence. Or equivalently, what is the optimal unitary that transforms a state to another state that possesses the maximal amount of coherence for a fixed reference basis. Here, by saying a state has the maximal coherence, we mean that its coherence cannot be enhanced by any unitary transformation, but it is not necessary to be maximally coherent [18]. In fact, for the relative entropy and squared $l_2$ norm of coherence, it has already been shown that the optimal bases are the mutually unbiased bases (MUBs), i.e., the bases mutually unbiased to the eigenbasis of the considered state [32]. A similar problem has also been discussed in Ref. [33], in which the authors defined the coherence measures by identifying the free operations as the maximally incoherent operations (MIOs), namely, $\Phi_{\text{MIO}}(\delta) = \mathcal{I}$, $\forall \delta \in \mathcal{I}$, and showed that the MUBs are optimal for any MIO monotone of coherence. Moreover, lower bounds for the relative entropy of coherence and the geometric coherence averaged over a set of MUBs were obtained [34]. Despite these progresses, it is noteworthy that there are non-MIO coherence monotones (e.g., the $l_1$ norm of coherence [35] and the coherence of formation [36]) and coherence measures that have not been proved to be a MIO monotone or not. Thus, it is worthwhile to identify the optimal bases and the corresponding maximally attainable coherence of them.

II. TECHNICAL PRELIMINARIES

The identification of an optimal basis for attaining the maximum coherence is equivalent to identifying an optimal unitary for which the transformed state has the maximum coherence in a fixed basis. As any density operator $\rho$ can always be diagonalized in the reference basis spanned by its eigenvectors, that is, by denoting $V = (|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_{d-1}\rangle)$, with $|\psi_i\rangle$ and $\lambda_i$ denoting, respectively, the eigenvectors and eigenval-
uses of $\rho$, we always have $V^\dagger V = \Lambda$, with
\[
\Lambda = \text{diag}\{\lambda_0, \lambda_1, \ldots, \lambda_{d-1}\},
\]
and we denote by $\tilde{U} = \tilde{U}_\Lambda V^\dagger$ the optimal unitary for a general state $\rho$, where $\tilde{U}_\Lambda$ is that for the diagonalized state $\Lambda$.

For the Hilbert space $\mathcal{H}$ of arbitrary dimension $d$, one of the MUB is given by $\{|\varphi^d_m\rangle\}$, with
\[
|\varphi^d_m\rangle = \frac{1}{\sqrt{d}} \sum_{n=0}^{d-1} e^{\frac{2\pi i}{d} mn} |n\rangle,
\]
where $i$ is the imaginary unit, and $m = 0, \ldots, d-1$. Moreover, for the case of $d$ being a prime, all the $d+1$ MUBs can be obtained. Apart from $\{|\varphi^d_m\rangle\}$ and $\{|\varphi^0_0\rangle = \sum_{m=0}^{d-1} \delta_{m0} |n\rangle\}$, the remaining $\{|\varphi^l_m\rangle\}$ for $l \in \{1, \ldots, d-1\}$ are \cite{37, 38}
\[
|\varphi^l_m\rangle = \frac{1}{\sqrt{d}} \sum_{n=0}^{d-1} e^{\frac{2\pi i}{d} stm \pi} |n\rangle.
\]

Then if we define the unitary operator
\[
U_{\text{mub}} = \sum_{m=0}^{d-1} |\varphi^k_m\rangle \langle m|,
\]
with $k \in \{1, \ldots, d\}$, the transformed state of the unitary operation $U_{\text{mub}}$ can be obtained as
\[
\tilde{\Lambda} = U_{\text{mub}} \Lambda U_{\text{mub}}^\dagger = \sum_{m=0}^{d-1} \lambda_m |\varphi^k_m\rangle \langle \varphi^k_m|,
\]
which is featured for the equal diagonal entries, and it is also called the contradiagonal density matrix in Ref. \cite{39}.

In general, one can consider the complex Hadamard matrix (CHM) described by \cite{40, 42}
\[
HH^\dagger = dI, |Hij| = 1 (\forall i, j = 0, \ldots, d-1),
\]
and for convenience of later presentation, we denote by $H_d = H/\sqrt{d}$ the rescaled CHM.

For any state eigenbasis $\{|\psi_i\rangle\}$, one can see from the above equations that the basis $\{U_{\text{mub}} |\psi_i\rangle\}$, or more general, the basis $\{H_d |\psi_i\rangle\}$, is mutually unbiased to $\{|\psi_i\rangle\}$. Due to this reason, when referring to MUBs in the following, we mean those bases mutually unbiased to $\{|\psi_i\rangle\}$.

### III. MAXIMUM COHERENCE IN THE MUBS

Based on the above preliminaries, we begin to identify the optimal basis for the maximum attainable coherence. There are two related concepts that need to be clarified. The first one is the maximally coherent state, which was defined to be a measure-independent state that can serve as a resource for generating all the other states in the same Hilbert space $\mathcal{H}$ by merely the IOs \cite{18}, and the second one is the maximal-coherence-value states (MCVSs), which have the maximal value of coherence \cite{43}. A general state in the optimal basis may not always be a maximally coherent state or a MCVS.

For the faithful measures of coherence, all the pure states have the maximum coherence in the MUBs, as for this case they belong to the set of MCVSs \cite{43}. For the relative entropy of coherence, which is a MIO monotone, the MUBs are also optimal, and the corresponding maximum is given by $\log_2 d - S(\rho)$, where $S(\rho) = -\text{tr}(\rho \log_2 \rho)$ denotes the von Neumann entropy \cite{32, 33, 44}. For the other coherence measures, we report our results in the following text.

We first consider the coherence measured by RoC \cite{13}. It was introduced based on the consideration that the mixture of $\rho$ with another state $\tau$ may be coherent or incoherent, and the minimal mixing required to destroy completely the coherence in $\rho$ is defined as the RoC. To be explicit, it is given by
\[
C_R(\rho) = \min_{\tau \in D(\mathbb{C}^d), \delta \in I} \left\{ s \geq 0 \left| \rho = \frac{\rho + s\tau}{1 + s} =: \delta \in I \right\},
\]
where $D(\mathbb{C}^d)$ is the convex set of density operators on $\mathcal{H}$, and $I$ is the set of incoherent states.

Starting from the above formula, we present our first result via the following theorem (see Appendix A for its proof).

**Theorem 1.** For state $\rho$ of dimension $d$, the maximum RoC attainable by optimizing the reference basis is
\[
C_R^{\text{max}}(\rho) = d\lambda_{\text{max}} - 1,
\]
where $\lambda_{\text{max}}$ is the largest eigenvalue of $\rho$. The bases mutually unbiased with the state eigenbasis are the optimal bases, and $U = H_d V^\dagger$ are the optimal unitaries.

While the RoC was defined as the minimal mixing required for destroying the coherence in a state \cite{13}, a similar measure called coherence weight was proposed recently \cite{20}. It reads
\[
C_w(\rho) = \min_{\delta \in I, \tau \in D(\mathbb{C}^d)} \left\{ s \geq 0 \left| \rho = (1 - s)\delta + s\tau \right\},
\]
which corresponds to the minimal weight factor $s$ of coherent state $\tau$ consumed for preparing $\rho$ on average. It obeys the four conditions for a faithful measure of coherence \cite{20}. Now, we show that the coherence weight also attains its maximum in the MUBs (see Appendix B for its proof).

**Theorem 2.** For state $\rho$ of dimension $d$, the maximum coherence weight attainable by optimizing the basis is
\[
C_w^{\text{max}}(\rho) = 1 - d\lambda_{\text{min}},
\]
where $\lambda_{\text{min}}$ is the smallest eigenvalue of $\rho$. The bases mutually unbiased with the state eigenbasis are the optimal bases, and $U = H_d V^\dagger$ are the optimal unitaries.

Third, we consider the Wigner-Yanase (WY) skew information measure of coherence. The primary measure defined using this quantity was given by \cite{27}
\[
\mathcal{I}(\rho, K) = -\frac{1}{2} \text{tr}\{[\sqrt{\rho}, K]^2\},
\]
with $K$ being an observable. But it was soon showed to violate the conditions for a faithful coherence measure \cite{45}. To avoid this problem, a modified version of coherence measure which
also uses the skew information was proposed \cite{21}. Compared with the original definition, it uses $|k\rangle\langle k|$ instead of $K$ as the observable and was defined as the summation of $I(\rho, |k\rangle\langle k|)$ over the basis vectors $\{|k\rangle\}$, i.e.,

$$C_{sk}(\rho) = \sum_k I(\rho, |k\rangle\langle k|), \quad (12)$$

while for the single-qubit state, it is qualitatively equivalent to the coherence measure $I(\rho, K)$ given in Ref. \cite{27}.

For this measure of coherence, we have the following theorem (see Appendix C for its proof).

**Theorem 3.** For state $\rho$ of dimension $d$, the maximum modified skew information measure of coherence attainable by optimizing the basis is

$$C_{sk}^{\text{max}}(\rho) = 1 - \frac{1}{d} \left( \sum_i \sqrt{\lambda_i} \right)^2, \quad (13)$$

where the bases mutually unbiased to the state eigenbasis are the optimal bases, and $U = H_d V^\dagger$ are the optimal unitaries.

It is noteworthy that $C_{sk}^{\text{max}}(\rho)$ equals the total coherence $C_I(\rho)$ presented in Ref. \cite{44}.

A major concern of any resource theory is how to manipulate the associated resource states. The above three theorems highlight the role of the MUBs (or equivalently, the unitaries given by the rescaled CHMs) on attaining the maximum coherence measured by the RoC, the coherence weight, and the WY skew information. This is of practical significance as the amount of coherence inherent within a state determines its capacity for quantum information processing \cite{2}. For example, in a quantum metrology task \cite{13}, $C_R(\rho)$ quantifies the maximum advantage achievable by using coherent probe $\rho$ as opposed to any incoherent probe $\delta$ \cite{13}.

The rescaled CHMs are optimal for attaining the maximum ROc and coherence weight can also be understood by combining Theorems 1 and 2 with the fact that $M$ (see Appendix A) is the coherence-value-preserving operation (CVPO) which conserves the coherence values of all states, or equivalently, any set of MCVSs is unchanged under CVPO \cite{43}. Consequently, provided that the basis $\{\phi_i^d\}$ is optimal, all the bases given by the equivalent class of CHMs are optimal. That is, by using $H_d V^\dagger$ any state can be transformed unitarily into another state that has the maximum attainable coherence. We noted that the RoC and the fidelity-based coherence measure are also MIO monotones as they are monotones of the special Rényi relative entropies \cite{46,47}, hence the finding that $H_d V^\dagger$ is optimal can also be understood from \cite{33}. But deriving the maximum attainable fidelity-based coherence is still a hard task for general states.

It is also noteworthy that Theorem 2 implies that the coherence weight for all the rank deficient states take the maximum 1 in the MUBs. Or equivalently, all the rank deficient states can be transformed unitarily into the MCVSs in the sense that $C_{sk}^{\text{max}}(\rho) = 1$ for them. This is a property of the coherence weight that differs it from the other coherence measures, as the latter are maximal only for the MCVSs given in Eq. (2) of Ref. \cite{43}. This also implies that the set of MCVSs may be different for different coherence measures.

Moreover, for the single qubit case, the MUBs are optimal for arbitrary coherence measure formulated in the framework of Baumgratz et al. \cite{18}. This can be proved by noting that the $l_1$ norm of coherence for a single qubit is $C_{l_1}(\rho) = (r_1^2 + r_2^2)^{1/2} \equiv r_{12}$, where $r_i = \text{tr}(\rho \sigma_i)$, and $\sigma_{1,2,3}$ are the Pauli operators. It implies that $r_{12}'$ for $\Phi_{l_1}(\rho)$ cannot be larger than $r_{12}$ for $\rho$ (see also \cite{48}). Meanwhile, by its definition we know that any IO monotone of coherence $C$ should not be increased by the IO. Then if $r_{12} \geq r_{12}'$, we always have

$$C(r_{12}) \geq C(r_{12}'). \quad (14)$$

On the other hand, $r_{12}$ is maximal in the MUBs for any single qubit state $\rho$, thus any IO monotone $C(\rho)$ attains its maximum value in the MUBs.

One can check the above result via all the known IO monotones of coherence such as the $l_1$ norm and relative entropy of coherence \cite{18}, the fidelity-based measure of coherence \cite{19}, the intrinsic randomness of coherence \cite{22}, the coherence of formation \cite{23}, and the coherence concurrence \cite{24}.

**IV. $l_1$ NORM OF COHERENCE**

The $l_1$ norm of coherence is $C_{l_1}(\rho) = \sum_{i \neq j} |\langle i | j \rangle|$, in the basis $\{|i\rangle\}$ \cite{18}, which is favored for the compact analytical solution. It was formulated in the framework of Baumgratz et al. \cite{18} and does not obey the additional conditions (C5) and (C6) presented in Ref. \cite{1}. It has been shown that $C_{l_1}(U \rho U^\dagger)$ is upper bounded by \cite{49}

$$B_d = \sqrt{(d^2 - d)/2|x|}, \quad (15)$$

where $x = (x_1, x_2, \ldots, x_{d-1})$ is the Bloch vector for $\rho$, with $x_i = \text{tr}(|i\rangle \langle i| \rho)$, and $\{X_i\}$ denoting generators of the Lie algebra SU($d$) \cite{50,51}.

The bound $B_d$ is intimately related to the quantumness captured by noncommutativity of the algebra of observables and the complementarity of quantum coherence under MUBs \cite{49}. It also has immediate consequence on quantum entanglement. This is because any bipartite entangled state must have a linear purity $\text{tr} \rho^2 \geq 1/(d - 1)$ \cite{52}, which is equivalent to $B_d \geq 1$. Hence, any bipartite entangled state must have the coherence larger than a critical value. Moreover, as $\text{tr} \rho^2 = 1/d + |x|^2/2$, and all the unitary operations $U$ do not change the mixedness $M(\rho) = d(1 - \text{tr} \rho^2)/(d - 1)$ of a state, one can give an alternative proof of the complementarity relation obtained in \cite{53} by using the bound $B_d$.

For any pure state and single-qubit state, it has been shown that the bound $B_d$ can always be reached, and the MUBs are the optimal reference bases. For general qutrit states, one can also show that the MUBs are optimal. This is because for $\tilde{A}$ of Eq. (5) with $d = 3$, we always have $C_{l_1}(\tilde{A}) = B_3$. As the bound $B_3$ cannot be exceed by any unitary equivalent states of $\tilde{A}$, the unitaries $U = H_d V^\dagger$ are optimal for any qutrit state.

For $d \geq 4$, $H_d V^\dagger$ is not optimal, in general \cite{32}. But one can see that for the family of physically allowed (i.e., $\rho_{\text{MCVS}} \geq ...$
with \( R = 2 \sqrt{1 - M_f/d} \), and \( M_f \) the mixedness of \( \rho_{\text{mcms}} \), the bound \( B_d \) is reached. Here, the phases \( \{ \phi_{ij} \} \) should satisfy the positive semidefinite constraints of \( \rho_{\text{mcms}} \). It covers the full set of maximally coherent mixed states (MCMSs). In [53], the authors stated that \( \{ \phi_{ij} \} \) can be removed by the incoherent unitary \( U = \sum_{n=0}^{d-1} e^{-i\phi_{n}[n]} |n\rangle \), with \( \phi_{ij} = \gamma_i - \gamma_j \). But apart from some very special cases, one can check directly that there does not exist such \( \{ \gamma_i \} \) in general. Consequently, \( \rho_m \), given in [53], is only a subset of the MCMSs.

Now, the question is whether there exists an optimal basis (or an optimal unitary \( U \)) such that the bound \( B_d \) is saturated for \( d \geq 4 \). We show through a counterexample that this is not always true. To this end, we consider the case of a rank-2 state \( \Lambda = \{ \lambda_0, \lambda_1, 0, 0 \} \). Then if there exists such an \( U \), it must transform \( \Lambda \) to \( \rho_{\text{mcms}} \) of Eq. (16). As the unitary transformation does not change the rank of a state, all of the third-order minors of \( \rho_{\text{mcms}} \) must be zero [54]. But this cannot always be satisfied. This is because for \( d = 4 \), \( \rho_{\text{mcms}} \) is incoherent unitary equivalent to

\[
\Lambda_U = \begin{pmatrix}
\frac{1}{4} & a & ae^{i\theta_1} & ae^{i\theta_2} \\
a & \frac{1}{4} & \frac{1}{4} & ae^{i\theta_3} \\
ae^{-i\theta_1} & \frac{1}{4} & a & ae^{i\theta_2} \\
ae^{-i\theta_2} & ae^{-i\theta_3} & \frac{1}{4} & a
\end{pmatrix},
\]

where \( a = R/2 \in [1/8, 1/4] \). The third-order leading principal minor can be calculated as

\[
D_3 = \frac{1}{64} - \frac{3}{4} a^2 + 2a^3 \cos \theta_1,
\]

from which we obtain \( \cos \theta_1 = 3/8a - 1/128a^3 \). Similarly, we have \( \cos \theta_3 = \cos \theta_1 \) (but \( \sin \theta_3 \) and \( \sin \theta_1 \) may be different). Further, the minor of the principal submatrix formed by removing from \( \Lambda_U \) its first row and last column is

\[
\Delta_3 = a^3 [1 + e^{-i(\theta_1 + \theta_2)}] - \frac{1}{4} a^2 (e^{-i\theta_1} + e^{-i\theta_2}) + \frac{1}{16} a^2 e^{-i\theta_2},
\]

and \( \Delta_3 = 0 \) yields

\[
e^{-i\theta_2} = \frac{16a^2 [1 + e^{-i(\theta_1 + \theta_2)}] - 4a (e^{-i\theta_1} + e^{-i\theta_2})}{1 - 16a^2}.
\]

But from Fig. 1 one can note that except the cases \( a = 1/4\sqrt{3} \) and \( 1/4 \), there are no solutions for \( \Delta_3 = 0 \). This implies that the rank-2 state \( \Lambda \) may not be transformed to a MCMS by any unitary, thus the bound \( B_d \) cannot always be reached.

Although \( B_d \) may not be reached in general, our numerical results present strong evidence that the difference between it and \( C_{l_1}^{\text{max}}(\Lambda) \) may be small. For the rank-2 state \( \Lambda \), we have performed calculations by choosing \( \lambda_0 = 0.05k \) (\( k \in \mathbb{Z} \)), and obtained the maximum \( C_{l_1}^{\text{max}}(\Lambda) \) via \( 10^9 \) equally distributed unitaries \( U \) generated according to the Haar measure [55, 56]. The results showed that the relative deviations of \( C_{l_1}^{\text{max}} \) from \( B_d \), i.e.,

\[
\frac{B_d - C_{l_1}^{\text{max}}}{B_d},
\]

are between \( 1.392836 \times 10^{-4} \) and \( 0.012743 \). It is also noteworthy that this deviation is upper bounded by \( 1 - O_d/B_d \).

In Fig. 2 we further showed the exemplified plots for states \( \Lambda = \text{diag}[0.1, 0.1, p, 0.8 - p], \text{diag}[0.04, 0.06, 0.1, p, 0.8 - p], \text{and} \text{diag}[0.02, 0.04, 0.06, 0.08, p, 0.8 - p] \), respectively. For comparison, we plotted in the same figure also the bound \( O_d \) given in Ref. [32], i.e.,

\[
O_d = \sum_{n=1}^{d-1} \sum_{i=0}^{d-1} \lambda_i^2 + \sum_{k \neq l}^{d-1} \lambda_k \lambda_l \cos \left( \frac{2\pi n}{d} (k - l) \right).
\]

From these plots one can see that in the regions of relative small \( p \), the two bounds \( O_d \) and \( B_d \) give nearly the same estimation for the maximally achievable \( l_1 \) norm of coherence. But with the increase of \( p \), \( C_{l_1}^{\text{max}} \) turns to violate those of \( O_d \), and are still very close to their upper bound \( B_d \). In the top-right insets of Fig. 2 we also plotted the relative deviations of \( C_{l_1}^{\text{max}} \) from \( B_d \). The results revealed that they are between \( 1.893424 \times 10^{-2} \) and \( 0.018391 \) for the considered data points. It is also expectable that with the increasing dimension \( d \), one should perform more and more runs of simulation to reduce the relative deviation due to the structure of the uniformly distributed Haar measure [55, 56]. This explains why the relative deviations are increased with \( d \) in general when the same runs of simulation are performed.

We have also calculated the distribution of \( C_{l_1}(U \Lambda U^\dagger) \) for \( p = 0.4 \) with \( 10^9 \) Haar distributed unitaries. The results were displayed in the insets at the bottom-left corner of Fig. 2. For \( d = 4, 5, \) and \( 6 \), the probabilities for \( C_{l_1}(U \Lambda U^\dagger) > O_d \) is about \( 57.65\%, 10.86\%, \) and \( 20.30\% \), respectively. This confirms again that \( O_d \) can be overcome for \( d \geq 4 \) [32]. In particular, the

FIG. 1: The absolute value of the right-hand side of Eq. (20) versus \( a \), with the sign of \( \sin \theta_1 \) and \( \sin \theta_3 \) being the same (the black solid line) and different (the red solid line).
FIG. 2: Maximum $l_1$ norm of coherence $C_{l_1}^{\text{max}}(\Lambda)$ for $d = 4, 5,$ and 6 (from top to bottom), where the black solid lines (red dashed lines) correspond to $O_d$ ($B_d$), and every blue solid circle was the numerical result obtained by $10^6$ equally distributed unitaries generated according to the Haar measure. Moreover, the insets at the top-right corner are the distribution of $C_{l_1}^{\text{max}}(\Lambda)$ from $B_d$, and the insets at the bottom-left corner are the distribution of $C_{l_1}^{\text{max}}(U\Lambda U^\dagger)$ for $p = 0.4$.

peak value of $C_{l_1}(U\Lambda U^\dagger)$ ($\sim 0.908$) is also larger than $O_4 \simeq 0.848528$ for $d = 4$. Of course, for the other two cases, the peak values ($\sim 1.415$ and $1.911$) turn out to be smaller than $O_6 \simeq 1.488135$ and $O_6 \simeq 1.961348$.

Finally, by combining Eq. (8) with the results of Refs. [13, 14], one can obtain another upper bound for the maximum $l_1$ norm of coherence, which is given by

$$R_d = (d - 1)(d\lambda_{\text{max}} - 1),$$

then it is natural to ask whether this bound could give a better estimation for $C_{l_1}^{\text{max}}$ than $B_d$. But a direct calculation shows that this is not the case. This is because for $\Lambda$ of Eq. (1), we always have $R_d \geq B_d$ (see Appendix D for its proof). Thus, the bound $R_d$ is not better than $B_d$.

V. SUMMARY

In summary, we have studied the maximal amount of quantum coherence attainable by optimizing the reference basis, or equivalently, by performing optimal unitary operations on the state in a fixed basis. For the RoC, the coherence weight, and the modified skew information measure of coherence, we obtained analytical solutions for their maximum values, and proved strictly that the optimal bases are the MUBs, i.e., the bases mutually unbiased with the eigenbasis of the considered state. Moreover, when considering the pure states and the single qubit states, the MUBs are optimal for any IO monotone of coherence. While these highlight role of the MUBs on attaining the maximum coherence, they fail for the $l_1$ norm of coherence for states $\rho$ of dimension $d \geq 4$. We emphasized the upper bound $B_d$ of $C_{l_1}(\rho)$, and showed that for the rank-2 state it may not always be reached. We also presented strong evidence that the difference between the maximum attainable $l_1$ norm of coherence and the bound $B_d$ may be small in most cases, though a strict proof is still needed.

By combining the present work with Refs. [32, 33, 44], it also seems that apart from the $l_1$ norm of coherence, most of the other well-known faithful coherence measures are maximal in the MUBs. Then there is an interesting question as to whether the coherence defined in the MUBs can be dubbed an intrinsic coherent property of quantum states? At least this can avoid the basis-dependent perplexity of various coherence measures, as in most cases we are inclined to scrutinize properties of a system via a basis-independent quantity.

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Appendix A: Proof of Theorem 1

By virtue of Eq. (7) one can see that when the mixture of $\tilde{\Lambda}$ and $\delta$ is incoherent, the required $\tilde{r}$ should be of the form $\tilde{r} = [(1 + s)\delta - \tilde{\Lambda}]/s$. The positive semidefiniteness of it requires $\langle \tilde{x}, \tilde{x} \rangle \geq 0, \forall \tilde{x} \neq 0$, where $\langle u, v \rangle = \text{tr}(u^\dagger v)$ is the inner product [54]. By choosing $\tilde{x} = (1, 1, \ldots, 1)^T$ (the superscript $T$ denotes transpose), assuming $\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_{d-1}$, and further using the relation

$$\langle \tilde{x}, |\phi_{m}^d\rangle \langle \phi_{m}^d |\tilde{x} \rangle = \begin{cases} d & \text{if } m = 0, \\ 0 & \text{if } m = 1, \ldots, d - 1, \end{cases}$$

5
one can derive
\[ \langle \tilde{x}, \tilde{\tau} \rangle = \frac{1}{s}(1 + s - d\lambda_0). \quad (A2) \]

Similarly, for \(|\phi_m^l\rangle\) with \(l = 1, \ldots, d - 1\), by defining \(\tilde{x}' = U_1^\dagger \tilde{x}\) with
\[ U_1 = \sum_{n=0}^{d-1} e^{-i \frac{2\pi}{d} mn^2} |n\rangle \langle n|, \]  
(A3)

one can show that the inner product \(\langle \tilde{x}', \tilde{\tau} \rangle\) is the same as Eq. (A2), then the positive semidefiniteness of \(\tilde{\tau}\) implies \(s \geq d\lambda_0 - 1\). As the RoC is defined to be the minimal weight of mixing, we have \(C_R(\lambda) \geq d\lambda_0 - 1\). This, together with the bound \(C_R(\lambda) \leq d\lambda_0 - 1\) given in [13], yields Eq. (8).

For the rescaled CHM, as one can always find an incoherent unitary \(M\) such that the entries in the first column of \(MHM^\dagger\) are 1. Then by denoting \(\tilde{x} = M^\dagger \tilde{x}\) and \(|\tilde{\varphi}_m\rangle\) the \(m\)th column of \(H_d\), one can show via Eq. (6) that \(\langle \tilde{x}', |\tilde{\varphi}_m\rangle \rangle\) is the same as Eq. (A2). Hence we still have \(s \geq d\lambda_0 - 1\), which further gives Eq. (8). This completes the proof.

Appendix B: Proof of Theorem 2

First, for every state \(\rho\) it holds that
\[ \rho \geq \lambda_{\min} I_d = d\lambda_{\min} \frac{I_d}{d}, \quad (B1) \]
with \(I_d/d\) being the maximally mixed state that is obviously incoherent. This, together with the alternative definition of the coherence weight \(C_w(\rho) = \min_{s \geq 0} \{s \geq 0 | \rho \geq (1 - s)\delta\} \geq 0\), implies immediately that
\[ C_w(\rho) \leq 1 - d\lambda_{\min}. \quad (B2) \]

Second, from Eq. (9) we know that for \(\tilde{\Lambda}\), the required \(\tilde{\tau}\) is \(\tilde{\tau} = [\tilde{\Lambda} - (1 - s)\delta]/s\), thus by assuming \(\lambda_0 \leq \lambda_1 \leq \ldots \leq \lambda_{d-1}\), \(\tilde{x} = (1, 1, \ldots, 1)^T\), and using Eq. (A1), we obtain
\[ \langle \tilde{x}, \tilde{\tau} \rangle = 1 + \frac{1}{s}(d\lambda_0 - 1). \quad (B3) \]

Then the positive semidefiniteness of \(\tilde{\tau}\) implies \(s \geq 1 - d\lambda_0\). Note that here we denote by \(\lambda_0\) the smallest eigenvalue, hence \(C_w(\tilde{\Lambda}) \geq 1 - d\lambda_{\min}\). By comparing this with Eq. (B2), we arrive at Eq. (10). Furthermore, with the help of the same \(\tilde{x}\) for proving Theorem 1, one can show that any general bases given by the rescaled CHMs are optimal for attaining the maximum coherence weight. This completes the proof.

Appendix C: Proof of Theorem 3

By using an equivalent definition of \(C_{sk}(\rho)\) \[ C_{sk}(\rho) = 1 - \sum_k \langle \psi_s | \psi_s \rangle \langle \psi_s | \psi_s \rangle, \quad (C1) \]

one can show that
\[ C_{sk}(U^\dagger U) = 1 - \sum_k \left( \sum_i \sqrt{\lambda_i} \langle \psi_i | \psi_i \rangle \langle \psi_i | \psi_i \rangle \right)^2 \]
\[ = 1 - \sum_k \left( \sum_i \sqrt{\lambda_i} \langle \psi_i | \psi_i \rangle \langle \psi_i | \psi_i \rangle \right)^2 \]
\[ \leq 1 - \frac{1}{d} \left( \sum_k \sum_i \sqrt{\lambda_i} \right)^2 \]
\[ = 1 - \frac{1}{d} \left( \sum_i \sqrt{\lambda_i} \right)^2, \quad (C2) \]

where \(\langle \psi_i | = U_i |\rangle\), and the overlap \(\tilde{k} = |\langle \psi_i |\rangle|\). The inequality comes from the fact that the arithmetic mean of a list of nonnegative real numbers is not larger than the quadratic mean of the same list, i.e.,
\[ \frac{1}{d} \sum_i a_i \leq \frac{1}{d} \sum_i a_i^2, \quad (C3) \]
and the last equality is due to \(\sum_k \tilde{k}^2 = 1, \forall i = 0, \ldots, d - 1\).

The equality condition in Eq. (C2) holds when \(\sum_i \sqrt{\lambda_i} k_i^2\) are the same for different \(k\), namely, when the basis \(\{|\psi_i\rangle\}\) is mutually unbiased to \(\{|k\rangle\}\). Clearly, \(H_d\) satisfies this requirement, as it gives \(|\langle \psi_i | k \rangle| = 1/\sqrt{d}, \forall i, k = 0, 1, \ldots, d - 1\). This completes the proof.

Appendix D: Proof of \(R_{\Delta} \geq B_{\Delta}\)

For state \(\Lambda\) of Eq. (11), by assuming \(\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_{d-1}\), we have
\[ R_\Delta^2 = (d - 1)^2 \left[ \sum_{j=1}^{d-1} \lambda_j^2 + \sum_{j=1}^{d-1} \lambda_j \right] - 2(d - 1) \lambda_0 \sum_{j=1}^{d-1} \lambda_j + 2 \sum_{i=1}^{d-1} \lambda_i \lambda_j, \quad (D1) \]
and
\[ B_\Delta^2 = (d - 1) \left[ \sum_{j=0}^{d-1} \lambda_j^2 - 2 \lambda_0 \sum_{j=1}^{d-1} \lambda_j \right] - 2 \sum_{i=1}^{d-1} \lambda_i \lambda_j, \quad (D2) \]
Then one can obtain directly that

\[ \mathcal{R}_d^2 - B_d^2 = d(d-1) \left[ (d-1)(d-2)\lambda_0^2 
- 2(d-2)\lambda_0 \sum_{j=1}^{d-1} \lambda_j + 2 \sum_{i=1<j}^{d-1} \lambda_i \lambda_j \right] \]

\[ = d(d-1) \sum_{i<j}^{d-1} (\lambda_0 - \lambda_i)(\lambda_0 - \lambda_j), \]

which implies \( \mathcal{R}_d \geq B_d. \)

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