Quantifying the coherence of pure quantum states

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(Dated: January 23, 2016)

In recent years, several measures have been proposed for characterizing the coherence of a given quantum state. We derive several results that illuminate how these measures behave when restricted to pure states. Notably, we present an explicit characterization of the closest incoherent state to a given pure state under the trace distance measure of coherence, and we affirm a recent conjecture that the ℓ_1 measure of coherence of a pure state is never smaller than its relative entropy of coherence. We then use our result to show that the states maximizing the trace distance of coherence are exactly the maximally coherent states, and we derive a new inequality relating the negativity and distillable entanglement of pure states.

PACS numbers: 03.67.Ac, 03.65.Ta, 02.30.Mv, 03.67.Mn

I. INTRODUCTION

One of the major goals in quantum information theory is to find effective ways of quantifying the amount of "quantumness" within a given system—that is, how much the system differs from any possible classical mechanical description of it. How this quantification is carried out varies heavily depending on context, however, as some quantum states might be useful for one quantum information processing task, yet useless for another.

When multiple quantum systems interact with each other, the resource of interest is typically *entanglement*, the quantification of which has been well-investigated over the past two decades [1–8]. However, when there is no interaction between different systems, the resource of interest is instead *coherence*, or the amount that a state is in a superposition of a given set of mutually orthogonal states. With roots in quantum optics [9, 10], coherence is an essential operational resource in quantum information processing, and has been shown to be intimately related to entanglement [11, 12]; in fact, it has been shown that one can measure coherence via entanglement [13].

Despite its usefulness, an effort to formalize the quantification of coherence has only begun somewhat more recently [14]. The defining properties of a *proper* coherence measure were identified in [15]; for example, a state ρ should have zero coherence under the proposed measure if and only if ρ is *incoherent* (i.e., it is diagonal in the pre-specified orthogonal basis, which we will always take to be the standard basis $\{|i\rangle\}_{i=1}^n$), since such states are exactly the ones that represent classical mixtures of the given basis states. We denote the set of all $n \times n$ matrices by $\mathcal{M}_n$, the set of density matrices by $\mathcal{D}_n$, and the set of incoherent states by $\mathcal{I}_n$, or simply $\mathcal{M}$, $\mathcal{D}$, and $\mathcal{I}$ if the dimension is irrelevant or clear from context.

The two most widely-known coherence measures are the ℓ_1-*norm of coherence*, defined as the sum of the absolute values of the off-diagonal entries of the density matrix:

$$C_{\ell_1}(\rho) := \sum_{i \neq j} |\rho_{ij}|,$$

and the *relative entropy of coherence* [14]:

$$C_{\mathrm{r}}(\rho) := S(\rho_{\mathrm{diag}}) - S(\rho),$$

where $S(\cdot)$ is the von Neumann entropy and ρ_{diag} is the state obtained from ρ by deleting all off-diagonal entries. Some other coherence measures that have been proposed recently include the *trace distance of coherence* [16], which is the trace norm distance to the closest incoherent state:

$$C_{\mathrm{tr}}(\rho) := \min_{\delta \in \mathcal{I}} \|\rho - \delta\|_{\mathrm{tr}} = \min_{\delta \in \mathcal{I}} \sum_{i=1}^{n} |\lambda_i(\rho - \delta)|,$$

where $\lambda_i(\rho - \delta)$ are the eigenvalues of the matrix $\rho - \delta$ and $\|\cdot\|_{\mathrm{tr}}$ is the trace norm, and the *robustness of coherence* [17]:

$$C_R(\rho) := \min_{\tau \in \mathcal{D}} \left\{ s \geq 0 \,\middle|\, \frac{\rho + s\tau}{1+s} \in \mathcal{I} \right\}.$$

The ℓ_1-norm of coherence, relative entropy of coherence, and robustness of coherence have all been shown to be proper coherence measures, and it has been shown that the trace distance of coherence is a proper measure of coherence when restricted to qubit states or X states [16]. Although the general case remains open, this partial result helps validate the fact that the trace distance is commonly used as a coherence measure. Additionally, simple formulas are known for all of these measures of coherence when restricted to pure states, except for the trace distance of coherence. Indeed, the ℓ_1-norm of coherence and the relative entropy of coherence are *defined* via explicit formulas, and the robustness of coherence of a pure state simply equals its ℓ_1-norm of coherence [17]. However, it was noted in [16] that it seems comparably difficult to compute the trace distance of coherence of a pure state, and evidence was given to suggest that a simple closed-form formula might not exist.

In this work, we thoroughly investigate how these measures of coherence behave on pure states. Our primary contribution in Section II is to give an "almost formula" for the trace distance of coherence of a pure state: we show that it is given by one of n different formulas (depending on the state), and which formula is the correct one can be determined simply by checking $\log_2(n)$ inequalities. We also completely characterize the closest incoherent state under the trace norm (and operator norm), and we present examples and MATLAB code to demonstrate the efficacy of our method both analytically and numerically. In Section III, we use our method to prove that the states maximizing the trace distance of coherence are exactly the maximally coherent states—another property that has already been known to hold for the other three measures of coherence. In Section IV, we prove a recent conjecture [16] that says that the ℓ_1 measure of coherence of a pure state is not smaller than its relative entropy of coherence, and as an immediate corollary we obtain an improvement to the known bound of the distillable entanglement of pure states in terms of their negativity. Finally, concluding remarks and open questions are discussed in Section V.

II. THE TRACE DISTANCE OF COHERENCE OF A PURE STATE

We now present a characterization of $C_{\rm tr}(|x\rangle\langle x|)$, where $|x\rangle \in \mathbb{C}^n$ is an arbitrary pure state (unit vector). Note that there is a diagonal unitary U and a permutation matrix P such that $PU|x\rangle$ is a unit vector having non-negative entries $x_1 \geq \cdots \geq x_n \geq 0$ in descending order. We then have

$$\||x\rangle\langle x| - \delta\|_{\rm tr} = \|PU(|x\rangle\langle x| - \delta)U^*P^t\|_{\rm tr}$$

for any $\delta \in \mathcal{I}$. So, we may replace $|x\rangle$ by $PU|x\rangle$. Without loss of generality, we will use this simplification to find the best approximation for $|x\rangle = (x_1, \ldots, x_n)^t$ with $x_1 \geq \cdots \geq x_n \geq 0$, but we note that it straightforwardly applies to the general setting of an arbitrary unit vector in $\mathbb{C}^n$.

With this modification, we have the following.

Theorem 1. *Suppose $|x\rangle = (x_1, \ldots, x_n)^t$ is a unit vector with entries $x_1 \geq \cdots \geq x_n \geq 0$. Let $s_\ell = \sum_{j=1}^{\ell} x_j$, $m_\ell = \sum_{j=\ell+1}^{n} x_j^2$, and $p_\ell = s_\ell^2 - 1 - \ell m_\ell$ for $\ell \in \{1, \ldots, n\}$. There is a maximum integer $k \in \{1, \ldots, n\}$ satisfying*

$$x_k > q_k := \frac{1}{2ks_k}\left(p_k + \sqrt{p_k^2 + 4km_ks_k^2}\right). \qquad (1)$$

The unique best approximation of $|x\rangle\langle x|$ in $\mathcal{I}$ with respect to the trace norm (and the operator norm) is $D = \mathrm{diag}(d_1, \ldots, d_k, 0, \ldots, 0) \in \mathcal{I}$ with

$$d_j = \frac{x_j - q_k}{s_k - kq_k} \quad \textit{for} \quad 1 \leq j \leq k.$$

Furthermore,

$$\begin{aligned} C_{\rm tr}(|x\rangle\langle x|) = \||x\rangle\langle x| - D\|_{\rm tr} &= 2(q_ks_k + m_k), \\ \textit{and} \qquad \||x\rangle\langle x| - D\| &= q_ks_k + m_k. \end{aligned}$$

Proof: We may assume that $x_n > 0$, and use continuity for the general case.

First, we prove that there exists a matrix $D = \mathrm{diag}(d_1, \ldots, d_k, 0, \ldots, 0)$ such that $|x\rangle\langle x| - D$ has an eigenvector $\mathbf{v} = (q_k, \ldots, q_k, x_{k+1}, \ldots, x_n)^t$ corresponding to its largest eigenvalue (we will later show that this D is the same one from the statement of the theorem). To this end, let $d_1, \ldots, d_k, q, \mu > 0$ be variables satisfying the matrix equation

$$(|x\rangle\langle x| - D)\mathbf{v} = \mu\mathbf{v} \quad \text{with} \quad \mathbf{v} = (q, \ldots, q, x_{k+1}, \ldots, x_n)^t.$$

Then $|x\rangle\langle x|\mathbf{v} = D\mathbf{v} + \mu\mathbf{v}$. Because $\langle x|\mathbf{v} = qs_k + m_k$, we have

$$\begin{aligned} &(qs_k + m_k)(x_1, \ldots, x_k, x_{k+1}, \ldots, x_n)^t \\ = \; &(d_1q + \mu q, \ldots, d_kq + \mu q, \mu x_{k+1}, \ldots, \mu x_n)^t. \end{aligned}$$

Summing up the first k entries of the vectors on the left and right sides, we have

$$(qs_k + m_k)s_k = k\mu q + q\sum_{j=1}^{k} d_j = k\mu q + q. \qquad (2)$$

Comparing the last $n-k$ entries of the vectors on both sides, we have

$$qs_k + m_k = \mu. \qquad (3)$$

Substituting (3) into (2) to eliminate μ, we have

$$f_k(q) := ks_kq^2 - q(s_k^2 - 1 - km_k) - s_km_k = 0. \qquad (4)$$

Letting q_k be the larger zero of $f_k(q)$, we have

$$q_k = \frac{1}{2ks_k}\left(p_k + \sqrt{p_k^2 + 4km_ks_k^2}\right) > 0,$$

where $p_k = s_k^2 - 1 - km_k$. Note that

$$q_1 = \left(\sqrt{1 - x_1^2} + x_1^2 - 1\right)/x_1 < x_1,$$

so there indeed exists a largest integer $k \in \{1, \ldots, n\}$ such that $x_k > q_k$. From this point forward, we fix k at this largest possible value, and we note that $s_k = x_1 + \cdots + x_k \geq kx_k \geq kq_k$. Define

$$d_j := (x_j - q_k)/(s_k - kq_k) > 0 \quad \text{for } j = 1, \ldots, k.$$

By our construction, we have

$$(|x\rangle\langle x| - D)\mathbf{v} = \mu\mathbf{v}.$$

Furthermore, by (3) we have

$$\begin{aligned} \||x\rangle\langle x| - D\| &= \mu = q_k s_k + m_k \quad \text{and} \\ \||x\rangle\langle x| - D\|_{\rm tr} &= 2\mu = 2(q_k s_k + m_k). \end{aligned}$$

Next, we will prove that $q_k \ge x_{k+1}$ if $k < n$. To this end, let $f_k(q)$ be the polynomial defined by (4). Then

$$\begin{aligned} & f_{k+1}(x_{k+1}) \\ =\ & (k+1)s_{k+1}x_{k+1}^2 - x_{k+1}[s_{k+1}^2 - 1 - (k+1)m_{k+1}] \\ & -s_{k+1}m_{k+1} \\ =\ & ks_k x_{k+1}^2 + kx_{k+1}^3 + s_{k+1}x_{k+1}^2 \\ & - x_{k+1}[s_k^2 + 2x_{k+1}s_k - 1 - k(m_k - x_{k+1}^2) - m_{k+1}] \\ & -(s_k + x_{k+1})(m_k - x_{k+1}^2) \\ =\ & ks_k x_{k+1}^2 - x_{k+1}(s_k^2 - 1 - km_k) - s_k m_k \\ & +s_{k+1}x_{k+1}^2 - 2s_{k+1}x_{k+1}^2 + x_{k+1}(m_k - x_{k+1}^2) \\ & -x_{k+1}m_k + s_{k+1}x_{k+1}^2 + x_{k+1}^3 \\ =\ & ks_k x_{k+1}^2 - x_{k+1}(s_k^2 - 1 - km_k) - s_k m_k \\ =\ & f_k(x_{k+1}). \end{aligned}$$

The product of the roots of the quadratic $f_k(q)$ equals $-s_k m_k$, which is negative, so they have opposite signs. As a result, for any positive number μ, $f_k(\mu) \le 0$ if and only if $\mu \le q_k$. Since we chose k so that $x_{k+1} \le q_{k+1}$ (recall that k is the largest subscript so that $x_k > q_k$), we have $f_{k+1}(x_{k+1}) \le 0$. It follows that $f_k(x_{k+1}) = f_{k+1}(x_{k+1}) \le 0$ as well, i.e., $x_{k+1} \le q_k$ as desired.

Finally, we will show that D is the (unique) best approximation of $|x\rangle\langle x|$ in $\mathcal{I}$ by establishing the following.

Claim. Assume $F = {\rm diag}\,(f_1, \ldots, f_n)$ such that $D - F \in \mathcal{I}_n$. Then $\mathbf{v}^* F \mathbf{v} \ge 0$.

To prove this claim, note that $D = {\rm diag}\,(d_1, \ldots, d_k, 0, \ldots, 0)$. If $D - F \in \mathcal{I}_n$, then $f_{k+1}, \ldots, f_n \le 0$. Hence

$$\begin{aligned} \mathbf{v}^* F \mathbf{v} &= \mathbf{v}^* {\rm diag}\,(f_1, \ldots, f_n)\mathbf{v} \\ &= \sum_{j=1}^k f_j q_k^2 + \sum_{j=k+1}^n f_j x_j^2 \\ &= -\sum_{j=k+1}^n f_j q_k^2 + \sum_{j=k+1}^n f_j x_j^2 \\ &= \sum_{j=k+1}^n f_j (x_j^2 - q_k^2) \ \ge\ 0, \end{aligned}$$

because we already showed that $q_k \ge x_{k+1} \ge \cdots \ge x_n$. By Proposition 2 in the Appendix, D is the best approximation element in $\mathcal{I}_n$ of $|x\rangle\langle x|$ with respect to the operator norm and the trace norm. This completes the proof of the claim.

To prove the uniqueness of D and k, suppose D_1 is another element in $\mathcal{I}$ such that $\||x\rangle\langle x| - D\| = \||x\rangle\langle x| - D_1\|$. Then

$$\begin{aligned} \||x\rangle\langle x| - D\| &= \min_{\delta \in \mathcal{I}} \||x\rangle\langle x| - \delta\| \\ &\le \||x\rangle\langle x| - (D + D_1)/2\| \\ &\le \|(|x\rangle\langle x| - D)/2\| + \|(|x\rangle\langle x| - D_1)/2\|. \end{aligned}$$

By [18, Proposition 1.2], there are unitary matrices $V_1, V_2 \in \mathcal{M}_n$ such that $V_1^*(|x\rangle\langle x| - D)V_2 = [\mu] \oplus Y$ and $V_1^*(|x\rangle\langle x| - D_1)V_2 = [\mu] \oplus Z$, where $Y, Z \in \mathcal{M}_{n-1}$ are negative semidefinite matrices, and $\||x\rangle\langle x| - D_1\| = \||x\rangle\langle x| - D\| = \mu$ is the largest eigenvalue of $|x\rangle\langle x| - D$ with eigenvector $\mathbf{v}$ as defined before. Hence, if $\mathbf{u}$ is the first column of V_2 and $\tilde{\mathbf{u}}$ is the first column of V_1, then $(|x\rangle\langle x| - D)\mathbf{u} = \mu\tilde{\mathbf{u}}$. It follows that $\mathbf{u} = \xi\mathbf{v}$ for some $\xi \in \mathbb{C}$ and $\tilde{\mathbf{u}} = \xi\mathbf{v}$. Consequently, $(|x\rangle\langle x| - D_1)\mathbf{v} = \mathbf{v}$, and $D\mathbf{v} = D_1\mathbf{v}$ implying that $D = D_1$ as $\mathbf{v}$ has positive entries. This contradicts the assumption that $D \ne D_1$. By Proposition 2 in the Appendix, we see that $D \in \mathcal{I}$ attains $\min_{\delta\in\mathcal{I}} \||x\rangle\langle x| - \delta\|$ if and only if D attains $\min_{\delta\in\mathcal{I}} \||x\rangle\langle x| - \delta\|_{\rm tr}$. Thus, D is the unique element in $\mathcal{I}$ attaining $C_{\rm tr}(|x\rangle\langle x|)$.

Because k is the rank of the unique best approximation of D in $\mathcal{I}$ (with respect to the operator norm), we see that k is unique, which completes the proof of the theorem. (Alternatively, if there is another $\tilde{k}$ satisfying (1), then one can use the construction in our proof to get $\tilde{D}$ of rank $\tilde{k}$ that best approximates $|x\rangle\langle x|$, which is a contradiction.) ☐

Before proceeding, we note that the $k = 1$ and $k = n$ cases of Theorem 1 actually simplify significantly:

Corollary 1. *Using the notation of Theorem 1, we have the following.*

1. *The best incoherent approximation of $|x\rangle\langle x|$ is a rank one matrix, which must equal* ${\rm diag}\,(1, 0, \ldots, 0)$*, if and only if $x_1 m_2 \ge 2x_2 m_1$.*
2. *The best incoherent approximation of $|x\rangle\langle x|$ is an invertible matrix, which must equal $D = {\rm diag}\,(d_1, \ldots, d_n) \in \mathcal{I}$ with*

$$d_j = \frac{1}{n}[1 - s_n(s_n - nx_j)] > 0 \quad \textit{for} \quad j = 1, \ldots, n,$$

if and only if $1 > s_n(s_n - nx_n)$.

Proof. To prove statement 1, we note that $k = 1$ if and only if $x_2 \le q_2$. This is equivalent to $0 \ge f_2(x_2)$, where $f_2(q)$ is the quadratic defined in (4), as shown in the proof of Theorem 1. Explicitly, we have

$$\begin{aligned} 0 \ \ge\ & 2s_2x_2^2 - x_2(s_2^2 - 1 - 2m_2) - s_2m_2 \\ =\ & 2(x_1 + x_2)x_2^2 - x_2[(x_1 + x_2)^2 - 1] + 2x_2m_2 - s_2m_2 \\ =\ & x_2[2(x_1 + x_2)x_2 - (x_1^2 + x_2^2 + 2x_1x_2 - 1)] \\ & +x_2m_2 - x_1m_2 \\ =\ & x_2[2x_2^2 + (1 - x_1^2 - x_2^2)] + x_2(1 - x_1^2 - x_2^2) - x_1m_2 \\ =\ & 2x_2m_1 - x_1m_2. \end{aligned}$$

To prove statement 2, note that $q_n = \frac{1}{ns_n}(s_n^2 - 1)$, and the stated inequality is equivalent to $d_j > 0$ for all j, which is to say that D is positive definite. ☐

Although Theorem 1 appears somewhat technical at first glance, it is very simple to use both numerically and analytically. On the numerical side, it provides an extremely fast algorithm for computing $C_{\rm tr}(|x\rangle\langle x|)$. Although it might seem somewhat time-consuming at first to find the value of k described by the theorem, the proof of the theorem showed that if $q_k < x_k$ then $q_j < x_j$ for all $j < k$. Thus we can search for k via binary search, which requires only $\log_2(n)$ steps, rather than searching through all n possible values of k. MATLAB code that implements this algorithm is available for download from [19], which is able to compute $C_{\rm tr}(|x\rangle\langle x|)$ for pure states $|x\rangle \in \mathbb{C}^{1,000,000}$ in under one second on a standard laptop computer. We contrast this with the naive semidefinite program for computing $C_{\rm tr}(|x\rangle\langle x|)$ [16], which can only reasonably handle states in $\mathbb{C}^{100}$ or so.

Theorem 1 can also be used to analytically compute $C_{\rm tr}(|x\rangle\langle x|)$ for arbitrary pure states as well, as we now demonstrate with some examples.

Example 1. *As a simple example, consider the qutrit pure state $|x\rangle = (2/3, 2/3, 1/3)$, which was investigated in [16]. A direct calculation reveals that*

$$\begin{aligned} q_1 &= \frac{1}{6}\big(3\sqrt{5}-5\big) \approx 0.2847, \\ q_2 &= \frac{1}{48}\big(3\sqrt{17}+5\big) \approx 0.3619, \quad \textit{and} \\ q_3 &= \frac{16}{45} \approx 0.3556. \end{aligned}$$

Thus $k = 2$ (since $q_1 < x_1$ and $q_2 < x_2$, but $q_3 \geq x_3$), which then gives $C_{\rm tr}(|x\rangle\langle x|) = \frac{1}{6}\big(3+\sqrt{17}\big)$ and $D = {\rm diag}(1/2, 1/2, 0)$, verifying that the state D found in [16] is indeed optimal.

Example 2. *As another example, consider an arbitrary qubit pure state $|x\rangle = (x_1, x_2) \in \mathbb{C}^2$. Then*

$$q_2 = \frac{|x_1x_2|}{|x_1|+|x_2|} \leq \min\{|x_1|, |x_2|\},$$

with equality if and only if either $x_1 = 0$ or $x_2 = 0$. If $x_1, x_2 \neq 0$ then $k = 2$ and we then have $C_{\rm tr}(|x\rangle\langle x|) = 2|x_1x_2|$ and $D = {\rm diag}(|x\rangle\langle x|)$, which agrees with the formula for qubit states found in [16]. If $x_1 = 0$ or $x_2 = 0$ then $k = 1$ and it is straightforward to check that we get the same formula.

III. MAXIMALLY COHERENT STATES UNDER THE TRACE NORM OF COHERENCE

We recall [15] that a pure state $|x\rangle \in \mathbb{C}^n$ is called *maximally coherent* if all of its entries have equal absolute value: $|x_1| = \cdots = |x_n| = 1/\sqrt{n}$. Recently it has been suggested that the maximum value of a proper measure of coherence should be attained exactly by the maximally coherent states [20], and this property is known to hold for the relative entropy of coherence (this is straightforward to prove, see [15] for example), the ℓ_1-norm of coherence [21, Theorem 2], and the robustness of coherence [17]. We now show that this same property also holds for the trace distance of coherence, which provides further evidence that it is indeed a proper measure of coherence.

Theorem 2. *For all (potentially mixed) states $\rho \in \mathcal{D}_n$, we have $C_{\rm tr}(\rho) \leq 2 - 2/n$. Furthermore, equality holds if and only if $\rho = |x\rangle\langle x|$, where $|x\rangle$ is a maximally coherent state.*

Proof. Let ρ be a general mixed state with spectral decomposition $\sum_{j=1}^n p_j|x_j\rangle\langle x_j|$ such that $p_1 \geq \cdots \geq p_k > 1/n \geq p_{k+1} \geq \cdots \geq p_n$. Then

$$\begin{aligned} \min_{\delta\in\mathcal{I}} \|\rho-\delta\|_{\rm tr} &\leq \|\rho - I/n\|_{\rm tr} \\ &= \sum_{j=1}^k (p_j - 1/n) + \sum_{j=k+1}^n (1/n - p_j) \\ &= 2\sum_{j=1}^k (p_j - 1/n) \\ &\leq 2(1-k/n) \\ &\leq 2(1-1/n), \end{aligned}$$

where the second equality holds because ${\rm tr}(\rho - I/n) = 0$. If the equality $\min_{\delta\in\mathcal{I}} \|\rho-\delta\|_{\rm tr} = 2(1-1/n)$ holds, then $k = 1$ so that $\rho = |x\rangle\langle x|$ has rank one, and $D = I/n$ satisfies $C_{\rm tr}(|x\rangle\langle x|) = \||x\rangle\langle x| - D\|_{\rm tr}$. We may replace $|x\rangle$ by $PU|x\rangle$ as in Section II and so we assume without loss of generality that $|x\rangle = (x_1, \ldots, x_n)^t$ with $x_1 \geq \cdots \geq x_n \geq 0$. By Corollary 1 (2), we see that $d_1 = \cdots = d_n$ so that $s_n - nx_1 = \cdots = s_n - nx_n$. Thus, $x_1 = \cdots = x_n$. The desired conclusion follows. □

IV. RELATIONSHIP BETWEEN THE ℓ_1-NORM OF COHERENCE AND THE RELATIVE ENTROPY OF COHERENCE

We now turn to Conjecture 6 of [16], which asserted that the ℓ_1-norm coherence of a pure state is never smaller than its relative entropy of coherence. This section is devoted to proving this conjecture. Before proceeding, recall that the relative entropy of coherence is defined in terms of the von Neumann entropy $S(\rho) := -{\rm tr}(\rho\log_2(\rho))$. From now on, we will write $\log = \log_2$ for notational simplicity, since we deal with no other base.

Theorem 3. *Suppose $\{\lambda_i\}_{i=1}^n$ are such that $\sum\limits_i \lambda_i = 1$ and $\lambda_i \geq 0$ for every i. Then*

$$-\sum_i \lambda_i \log\lambda_i \leq \Big(\sum_i \sqrt{\lambda_i}\Big)^2 - 1.$$

Proof. In order to prove the above inequality, it suffices to show that the function $f(\vec{\lambda}) := (\sum\limits_i \sqrt{\lambda_i})^2 - 1 + \sum\limits_i \lambda_i \log\lambda_i$ is always non-negative for any probability vector $\vec{\lambda}$.

Without loss of generality, we can assume $0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n \leq 1$. Let λ_i to be the smallest one such that $\lambda_i > 0$, and consider the following perturbation:

$$\begin{aligned}
& f\big((\lambda_1, \cdots, \lambda_{i-1}, \lambda_i - \epsilon, \lambda_{i+1}, \cdots, \lambda_{n-1}, \lambda_n + \epsilon)\big) \\
& -f\big((\lambda_1, \cdots, \lambda_n)\big) \\
= \ & \big(\sum_{j \neq i,n} \sqrt{\lambda_j} + \sqrt{\lambda_i - \epsilon} + \sqrt{\lambda_n + \epsilon}\big)^2 \\
& -\big(\sum_{j \neq i,n} \sqrt{\lambda_j} + \sqrt{\lambda_i} + \sqrt{\lambda_n}\big)^2 \\
& +(\lambda_i - \epsilon)\log(\lambda_i - \epsilon) + (\lambda_n + \epsilon)\log(\lambda_n + \epsilon) \\
& -\lambda_i \log \lambda_i - \lambda_n \log \lambda_n \\
= \ & \big(2 \sum_{j \neq i,n} \sqrt{\lambda_j} + \sqrt{\lambda_i - \epsilon} + \sqrt{\lambda_n + \epsilon} + \sqrt{\lambda_i} + \sqrt{\lambda_n}\big) \\
& \times\big(\sqrt{\lambda_i - \epsilon} + \sqrt{\lambda_n + \epsilon} - \sqrt{\lambda_i} - \sqrt{\lambda_n}\big) \\
& +\lambda_i \log\big(1 - \frac{\epsilon}{\lambda_i}\big) + \lambda_n \log\big(1 + \frac{\epsilon}{\lambda_n}\big) \\
& +\epsilon[\log(\lambda_n + \epsilon) - \log(\lambda_i - \epsilon)].
\end{aligned}$$

Recall that $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + O(x^3)$ and $\log(1+x) = x - \frac{x^2}{2} + O(x^3)$, the above expression simplifies as

$$\begin{aligned}
& \left[2 \sum_{j \neq i,n} \sqrt{\lambda_j} + \sqrt{\lambda_i}\big(2 - \frac{\epsilon}{2\lambda_i}\big) + \sqrt{\lambda_n}\big(2 + \frac{\epsilon}{2\lambda_n}\big)\right] \\
& \times \left(-\frac{\sqrt{\lambda_i}\epsilon}{2\lambda_i} + \frac{\sqrt{\lambda_n}\epsilon}{2\lambda_n}\right) + O(\epsilon^2) \\
= \ & \big(\sum_j \sqrt{\lambda_j}\big)\left(\frac{1}{\sqrt{\lambda_n}} - \frac{1}{\sqrt{\lambda_i}}\right)\epsilon + O(\epsilon^2).
\end{aligned}$$

So, if $0 < \lambda_i < \lambda_n$, we will have

$$\begin{aligned}
& f((\lambda_1, \cdots, \lambda_{i-1}, \lambda_i - \epsilon, \lambda_{i+1}, \cdots, \lambda_{n-1}, \lambda_n + \epsilon)) \\
< \ & f((\lambda_1, \cdots, \lambda_n)).
\end{aligned}$$

In other words, if f achieves its minimum at $(\lambda_1, \cdots, \lambda_n)$, then all its positive entries must be identical, i.e. $(\lambda_1, \cdots, \lambda_n) = (0, \cdots, 0, \frac{1}{k}, \cdots, \frac{1}{k})$, in which case $f(\lambda) = k - 1 + \log\frac{1}{k} = k - 1 - \log k$, which is always non-negative for $k \in \mathbb{Z}^+$. The result follows. □

Corollary 2. *For every pure state $|x\rangle$,*

$$C_{\ell_1}(|x\rangle\langle x|) \geq \max\{C_r(|x\rangle\langle x|), 2^{C_r(|x\rangle\langle x|)} - 1\}.$$

Proof. Write $|x\rangle = \sum_{i=1}^n \sqrt{\lambda_i}|i\rangle$ for a given basis $\{|i\rangle\}_{i=1}^n$. Then $C_{\ell_1}(|x\rangle\langle x|) = \big(\sum_{i=1}^n \sqrt{\lambda_i}\big)^2 - 1$. Recall that the von Neumann entropy is zero for pure states, and so $C_r(|x\rangle\langle x|)$ reduces to $S(|x\rangle\langle x|_{\text{diag}}) = -\sum_{i=1}^n \lambda_i \log \lambda_i$. In [16, Proposition 5], the authors prove that $C_{\ell_1}(|x\rangle\langle x|) \geq 2^{C_r(|x\rangle\langle x|)} - 1$. Theorem 3 above states that $C_{\ell_1}(|x\rangle\langle x|) \geq -\sum_{i=1}^n \lambda_i \log \lambda_i = C_r(|x\rangle\langle x|)$. □

We note that Corollary 2 improves the bound $C_{\ell_1}(|x\rangle\langle x|) \geq \ln(2)C_r(|x\rangle\langle x|)$ given in [16, Proposition 5]. We also note, following the discussion in [16, Section III], that Corollary 2 improves a well-known inequality relating the negativity [22] and the distillable entanglement of pure states.

To elaborate a bit, we recall that a well-known upper bound on the relative entropy of entanglement $E_r(|y\rangle\langle y|)$ of a pure state $|y\rangle \in \mathbb{C}^m \otimes \mathbb{C}^n$ in terms of its negativity $N(|y\rangle\langle y|)$ is $E_r(|y\rangle\langle y|) \leq \log(1 + 2N(|y\rangle\langle y|))$. Since the relative entropy of entanglement is equal to the distillable entanglement when restricted to pure states, the same inequality holds for distillable entanglement as well. Using our results, we immediately obtain the following improvement to this bound:

Corollary 3. *For every pure state $|y\rangle \in \mathbb{C}^m \otimes \mathbb{C}^n$,*

$$E_r(|y\rangle\langle y|) \leq 2N(|y\rangle\langle y|).$$

Proof. It is straightforward to verify that if $|x\rangle = \sum_{i=1}^n x_i|i\rangle$ and $|y\rangle$ has Schmidt coefficients $\{x_i\}_{i=1}^n$, then $C_{\ell_1}(|x\rangle\langle x|) = 2N(|y\rangle\langle y|)$ and $C_r(|x\rangle\langle x|) = E_r(|y\rangle\langle y|)$. Thus using Corollary 2 immediately implies that

$$E_r(|y\rangle\langle y|) \ = \ C_r(|x\rangle\langle x|) \leq C_{\ell_1}(|x\rangle\langle x|) = 2N(|y\rangle\langle y|),$$

as desired. □

It is straightforward to verify that the bound provided by Corollary 3 is strictly better than the known bound $E_r(|y\rangle\langle y|) \leq \log(1 + 2N(|y\rangle\langle y|))$ exactly when $N(|y\rangle\langle y|) < 1/2$.

V. CONCLUSIONS AND DISCUSSION

In this work, we derived an explicit expression for the trace distance of coherence of a pure state, as well as the closest incoherent state to a given pure state with respect to the trace distance. One natural question that arises from this work is whether or not Theorem 1 can be used to show that the trace distance of coherence is strongly monotonic under incoherent quantum channels (and is thus a proper coherence measure), at least when it is restricted to pure states. We also proved that the states maximizing the trace distance of coherence are exactly the maximally coherent states, which provides evidence in favor of it being a proper coherence measure.

We also proved that the ℓ_1-norm of coherence is not smaller than the relative entropy of coherence for pure states (Corollary 2), and used this result to derive a new relationship between negativity and distillable entanglement of pure states. However, we note that it has been conjectured that the same relationship between the ℓ_1-norm of coherence and the relative entropy of coherence holds even for arbitrary mixed states. This more general conjecture is beyond the scope of our work, though; our perturbation techniques for the case of pure states rely on the linearity of the first-order term, which is no longer linear for the mixed state case. Perturbation techniques may still apply if we study higher-order terms, however, more detailed calculation may be involved.

ACKNOWLEDGEMENTS

The authors would like to thank Diana Pelejo and Yue Liu for some helpful comments in the early discussion of the project. C.-K.L. is an affiliate member of the Institute for Quantum Computing, University of Waterloo. He is an honorary professor of the University of Hong Kong and the Shanghai University. His research was supported by USA NSF grant DMS 1331021, Simons Foundation Grant 351047, and NNSF of China Grant 11571220. S.P. was supported by NSERC Discovery Grant number 1174582.

[1] C. H. Bennett, D. P. Di Vincenzo, J. Smolin, and W. K.Wootters, Phys. Rev. A **54**, 3824 (1996).
[2] F. G. S. L. Brandão, Phys. Rev. A **72**, 022310 (2005).
[3] P. Hayden, M. Horodecki, and B. Terhal, J. Phys. A: Math. Gen. **34**, 6891–6898 (2001).
[4] M. Horodecki, Quantum Inf. Comput. **1**, 3 (2001).
[5] E. M. Rains, Phys. Rev. A **60**, 173 (1999); 63, 173(E) (1999).
[6] A. Shimony, Ann. N.Y. Acad. Sci., **755**, 675–679 (1995).
[7] M. Steiner, Phys. Rev. A **67**, 054305 (2003).
[8] G. Vidal and R. Tarrach, Phys. Rev. A **59**, 141 (1999).
[9] R. J. Glauber, Phys. Rev. **131**, 2766 (1963).
[10] E.C.G. Sudarshan, Phys. Rev. Lett. **10**, 277 (1963).
[11] Y. Yao, X. Xiao, L. Ge, and C.P. Sun, Phys. Rev. A **92**, 022112 (2015).
[12] X. Yuan, H. Zhou, Z. Cao, and X. Ma, Phys. Rev. A **92**, 022124 (2015).
[13] A. Streltsov, U. Singh, H.S. Dhar, M.N. Bera, and G. Adesso, Phys. Rev. Lett. **115**, 020403 (2015).
[14] J. Åberg, *Quantifying superposition* (2006), preprint available at: http://arxiv.org/abs/quant-ph/0612146
[15] T. Baumgratz, M. Cramer, and M. B. Plenio, Phys. Rev. Lett. **113**, 140401 (2014).
[16] S. Rana, P. Parashar, and M. Lewenstein, Phys. Rev. A **93**, 012110 (2016).
[17] C. Napoli, T. R. Bromley, M. Cianciaruso, M. Piani, N. Johnston, and G. Adesso. *Robustness of coherence: An operational and observable measure of quantum coherence* (2016), preprint available at: http://arxiv.org/abs/1601.03781
[18] C.K. Li, C.M. Cheng and R.A. Horn, Linear Algebra Appl. **341**, 219–237 (2002).
[19] MATLAB code available with the arXiv preprint of this manuscript, see “other formats” of this manuscript.
[20] Y. Peng, Y. Jiang, and H. Fan, *Maximally coherent states and coherence-preserving operations* (2015), preprint available at: http://arxiv.org/abs/1511.02576
[21] U. Singh, M.N. Bera, H.S. Dhar, and A.K. Pati, Phys. Rev. A **91**, 052115 (2015).
[22] G. Vidal and R. F. Werner, Phys. Rev. A **65**, 032314 (2002).
[23] I. Singer, *The theory of best approximation and functional analysis*, CBMS-NSF Regional Conf. Ser. in Appl. Math. **13**, SIAM, Philadelphia, PA (1974).

Appendix: Some approximation theory results

In this section we present some of the technical results that we needed in the proofs of Theorems 1 and 2. We begin with a general result in approximation theory; for example, see [23].

Proposition 1. *Suppose W is a closed convex set of a finite dimensional normed space $(V, ||| \cdot |||)$, and $\mathbf{v} \in V - W$. Then $\mathbf{w} \in W$ is the best approximation of $\mathbf{v}$ if and only if there is a linear functional f with $|||f|||^* \le 1$ such that $f(\mathbf{v}-\mathbf{w}) = |||\mathbf{v}-\mathbf{w}|||$ and $f(\mathbf{z}) \ge 0$ for all $\mathbf{z} \in V$ such that $\mathbf{w}-\mathbf{z} \in W$.*

If $||| \cdot |||$ is a norm on $\mathbb{C}^n$, the linear functional f in the above proposition has the form $f(X) = \mathrm{tr}\,(MX)$ for some M in the dual norm ball of $||| \cdot |||$. It is well known that the norms $\|\cdot\|_{\rm tr}$ and $\|\cdot\|$ are dual to each other, and their respective norm balls equal

$$\begin{aligned} \mathcal{B}_{\rm tr} &= \{A \in \mathbb{C}^n : \|A\|_{\rm tr} \le 1\} \\ &= \mathrm{conv}\,\{\pm \mathbf{u}\mathbf{u}^* : \mathbf{u} \text{ is a unit vector in } \mathbb{C}^n\}, \text{ and} \\ \mathcal{B} &= \{A \in \mathbb{C}^n : \|A\| \le 1\} \\ &= \mathrm{conv}\,\{A \in \mathbb{C}^n : A \text{ is unitary}\}. \end{aligned}$$

By Proposition 1 and the above fact, we have the following result for pure states.

Proposition 2. *Let $|x\rangle \in \mathbb{C}^n$ be a unit vector such that $|x\rangle\langle x| \in \mathcal{D}_n - \mathcal{I}$, and $\delta \in \mathcal{I}$. Then $|x\rangle\langle x| - \delta$ has exactly one positive eigenvalue λ_1, and*

$$\||x\rangle\langle x| - \delta\|_{\rm tr} = 2\||x\rangle\langle x| - \delta\| = 2\lambda_1.$$

Consequently, the following conditions are equivalent for a matrix $D \in \mathcal{I}$.

(a) $\||x\rangle\langle x| - D\|_{\rm tr} = \min\{\||x\rangle\langle x| - \delta\|_{\rm tr} : \delta \in \mathcal{I}\}$.

(b) $\||x\rangle\langle x| - D\| = \min\{\||x\rangle\langle x| - \delta\| : \delta \in \mathcal{I}\}$.

(c) *If $\mathbf{v}$ is the eigenvector corresponding to the unique positive eigenvalue of $|x\rangle\langle x| - D$, then $\mathbf{v}^* F \mathbf{v} \ge 0$ for any diagonal matrix F such that $D - F \in \mathcal{I}$.*

Proof. Note that if $|x\rangle\langle x|$ is not a diagonal matrix, then $|x\rangle\langle x| - \delta$ has eigenvalues $\lambda_1 > 0 \ge \lambda_2 \ge \cdots \ge \lambda_n$ by Weyl's inequality. Because $\mathrm{tr}\,(|x\rangle\langle x| - \delta) = \sum_{j=1}^n \lambda_j = 0$, we have $\||x\rangle\langle x| - \delta\| = \lambda_1$ and $\||x\rangle\langle x| - \delta\|_{\rm tr} = \lambda_1 - \sum_{j=2}^n \lambda_j = 2\lambda_1$ So, the first assertion, and the equivalence of (a) and (b) follow. In particular, the same matrix D minimizes the trace norm and the operator norm.

A matrix $D \in \mathcal{I}$ is best approximation of $|x\rangle\langle x|$ with respect to the $\|\cdot\|_{\rm tr}$ if an only if there is an element H in the dual norm ball of $\|\cdot\|$ such that $\mathrm{tr}\,(|x\rangle\langle x| - D)H = \||x\rangle\langle x| - D\|$ and $\mathrm{tr}\,(HF) \ge 0$ for any F such that $D - F \in \mathcal{I}$. If H has spectral decomposition $\sum_{j=1}^n \xi_j \mathbf{u}_j \mathbf{u}_j^*$, then $\mathrm{tr}\,(|x\rangle\langle x| - D)H = \lambda_1$ can happen if and only if $H = \mathbf{v}\mathbf{v}^*$. □

For mixed states, we have the following results, which are not used in our paper but may be useful for future study.

Proposition 3. *Let $A \in \mathcal{D}_n$. The following conditions are equivalent.*

(a) $\|A - D\|_{\rm tr} = \min\{\|A - \delta\|_{\rm tr} : \delta \in \mathcal{I}\}$.

(b) *There is a contraction $H \in \mathbb{C}^n$ such that* $\mathrm{tr}\,((A - D)H) = \|A - D\|_{\rm tr}$ *and* $\mathrm{tr}\,(FH) \geq 0$ *for any diagonal matrix F satisfying $D - F \in \mathcal{I}_n$.*

(c) *There is a unitary $U \in \mathcal{M}_n$ such that $U^*(A - D)U = X_1 \oplus -X_2 \oplus 0_{n-p-q}$, where $X_1 \in \mathcal{M}_p, X_2 \in \mathcal{M}_q$ are diagonal matrices with positive diagonal entries, and a contraction $X_3 \in \mathcal{M}_{n-p-q}$ such that* $\mathrm{tr}\,((I_p \oplus -I_q \oplus X_3)UFU^*) \geq 0$ *for any diagonal matrix F satisfying $D - F \in \mathcal{I}_n$.*

Proof. By Proposition 1 and the remark after it, condition (a) holds if and only if there is H in the dual norm ball of the trace norm satisfying condition (b).

We can obtain more information about the matrix H in condition (b). Clearly, if $A - D$ has spectral decomposition $\sum_{j=1}^{p} \mu_j \mathbf{u}_j \mathbf{u}_j^* - \sum_{j=1}^{q} \nu_j \mathbf{v}_j \mathbf{v}_j^*$, where

$$\mu_1, \ldots, \mu_p, \nu_1, \ldots, \nu_q > 0,$$

then

$$H = \sum_{j=1}^{p} \mathbf{u}_j \mathbf{u}_j^* - \sum_{j=1}^{q} \mathbf{v}_j \mathbf{v}_j^* + \sum_{j=1}^{n-p-q} \xi_j \mathbf{z}_j \mathbf{z}_j^*,$$

so that $\{\mathbf{u}_1, \ldots, \mathbf{u}_p, \mathbf{v}_1, \ldots, \mathbf{v}_q, \mathbf{z}_1, \ldots, \mathbf{z}_{n-p-q}\}$ is an orthonormal basis for $\mathbb{C}^n$. Let U be the unitary matrix whose columns are precisely these basis vectors. We then get condition (c). If (c) holds, one can let $H = U^*(I_p \oplus -I_q \oplus X_3)U$. Then condition (b) holds. □

Remark If the best approximation element $D \in \mathcal{I}$ to A is such that $A - D$ is invertible, then $p + q = n$, and we have a Hermitian unitary H satisfying the optimality condition.

Using a similar argument, we have the following.

Proposition 4. *Let $A \in \mathcal{D}_n$. The following are equivalent.*

(a) $\|A - D\| = \min\{\|A - \delta\| : \delta \in \mathcal{I}\}$.

(b) *There is rank r orthogonal projection $P \in \mathcal{M}_n$ satisfying $|\mathrm{tr}\,((A - D)P)| = \|A - D\|$, where r is the number of non-zero eigenvalues of $A - D$, such that $\mathrm{tr}\,(PF) \geq 0$ for any diagonal matrix F satisfying $D - F \in \mathcal{I}_n$.*