Converting multilevel nonclassicality into genuine multipartite entanglement

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Abstract
Characterizing genuine quantum resources and determining operational rules for their manipulation are crucial steps to appraise possibilities and limitations of quantum technologies. Two such key resources are nonclassicality, manifested as quantum superposition between reference states of a single system, and entanglement, capturing quantum correlations among two or more subsystems. Here we present a general formalism for the conversion of nonclassicality into multipartite entanglement, showing that a faithful reversible transformation between the two resources is always possible within a precise resource-theoretic framework. Specializing to quantum coherence between the levels of a quantum system as an instance of nonclassicality, we introduce explicit protocols for such a mapping. We further show that the conversion relates multilevel coherence and multipartite entanglement not only qualitatively, but also quantitatively, restricting the amount of entanglement achievable in the process and in particular yielding an equality between the two resources when quantified by fidelity-based geometric measures.

1. Introduction

Signature features of the quantum world have been recently recognized as resources that can be harnessed for disruptive technologies \([1]\). One such resource, embodying the nonclassicality of quantum mechanics, is the possibility for a quantum system to exist in a superposition of 'classical' states. The latter are usually determined based on physical considerations; for instance, in continuous-variable systems they can be identified with the Glauber–Sudarshan coherent states \([2, 3]\), while in discrete-variable systems they can be taken to form a reference orthonormal basis (e.g. the energy eigenbasis), so that superposition manifests as quantum coherence \([4–12]\).

Superposition underlies other nonclassical phenomena such as quantum correlations among parts of a quantum system \([13, 14]\). In particular, entanglement is itself a key resource and a characteristic trait of quantum mechanics, and stems from the superposition principle in conjunction with the tensor product structure associated to composite systems. Despite the common origin, entanglement and superposition can be formalized according to different resource theories: the former being tied to the paradigm of spatially separated laboratories which can only implement local operations and classical communication (LOCC) for free \([13]\), while the second specified by the inability to create superpositions of the classical states for free \([4, 7, 12, 15, 16]\). Consequently, these two resources, like two currencies, enjoy different uses in quantum technologies. It thus becomes particularly relevant to investigate the connection between these two types of resource beyond a merely conceptual standpoint, and to devise operational schemes that allow the dynamical transformation of one into the other.
Several works have analyzed this problem. In quantum optics, nonclassicality gets mapped into entanglement by a beam splitter [17–21], while, in the discrete-variable scenario, it is the controlled NOT (CNOT) gate [22, 23] that plays a similar role. The quantitative interplay between the degree of nonclassicality and the bipartite entanglement obtained from it has been investigated as well [15, 16, 20, 24–27]. These studies have advanced our understanding of nonclassicality as a resource in systems of arbitrary dimension [7, 12, 15, 16, 25–32].

In this paper, we investigate the conversion of nonclassicality, expressed as superposition between multiple levels of a quantum system, into multipartite entanglement. In section 2 we show that there always exists a state-independent unitary mapping, realized by operations which alone cannot create nonclassicality, such that the presence of \( k \)-level nonclassicality in the state of a single \( d \)-level system is necessary and sufficient to create \( k + 1 \)-partite entanglement between the system and \( k \) ancillas.

To exemplify such a conversion procedure, in section 3 we specialize to quantum coherence as an instance of nonclassicality [12], and introduce an explicit physical protocol which directly converts \( k \)-level coherence into \( k + 1 \)-body multipartite entanglement. The protocol entangles a \( d \)-level system (qudit) with up to \( d \) qubits by a sequential application of generalized CNOT gates (free operations in the resource theory of coherence formalized in [7, 9]). The protocol can be further extended via the decoupling of the qudit system by LOCC (free operations in the resource theory of entanglement [13]), to provide a mapping of \( k \)-coherence into multipartite entanglement of the ancillary qubits alone. This process can also be seen as a toy model for decoherence [33] due to the interaction with a many-body environment, with information about the superposition leaking into the environment in the form of multipartite entanglement.

Finally, in section 4 we show that the initial amount of \( k \)-coherence places a quantitative restriction on the amount of entanglement that can be converted from it. In particular, the fidelity-based geometric measure of \( k + 1 \)-partite entanglement [34, 35] at the output of the protocol is exactly equal to the fidelity-based geometric measure of \( k \)-coherence in the input state of the \( d \)-level system—a computable quantifier of multi-level coherence introduced here, extending previous work in [7, 26].

2. Nonclassicality conversion

Nonclassicality is a notion that depends on the preassigned set of states that are deemed ‘classical’. Choosing a finite set of states \( \{ \ket{\chi_i} \} \) which spans the whole Hilbert space \( \mathcal{H} \) to constitute the pure classical states, as dictated by the physics of the problem under investigation, one asks whether a mixed state \( \rho \) can be represented as a convex combination of classical states only. If this is not possible—that is, if one has to consider superpositions of \( \{ \ket{\chi_i} \} \)—then \( \rho \) is a nonclassical state. In other terms, the set of all classical states \( \mathcal{C} \) is formed by the convex hull of \( \{ \ket{\chi_i} \} \).

For finite-dimensional systems, the notion of nonclassicality is often understood as quantum coherence [4, 7, 12]. However, following [15, 16], we note that the approach presented here is more general, since one does not require the states \( \{ \ket{\chi_i} \} \) to be orthogonal. This provides a common framework applicable e.g. to classical sets formed by SU(\( N \)) Gilmore–Perelomov coherent states [36, 37] in discrete-variable systems and Glauber–Sudarshan coherent states [2, 3] in continuous-variable systems, which are not orthogonal yet such that any finite subset thereof is linearly independent [25].

The framework adopted here leads to a natural measure of the level of nonclassicality of a state. For a pure state, one can indeed define the nonclassical rank \( R_N \) [15, 24] as \( R_N(\ket{\psi}) = \min \{ r \mid \ket{\psi} = \sum_{i=1}^{r} c_i \ket{\chi_i}, \ket{\chi_i} \in \mathcal{C} \} \), with nonzero complex coefficients \( c_i \). This clearly resembles the definition of the Schmidt rank \( R_S(\ket{\psi}) \) of bipartite entangled states [38], and it can be extended to mixed states in the same way as the the Schmidt rank is extended to the Schmidt number \( N_S \) [39]. We thus define the nonclassical number \( N_N \) of a mixed state \( \rho \) as \( N_N(\rho) = \min_{\rho(\ket{\psi})} \max_{\ket{\psi}} R_N(\ket{\psi}) \), where the minimization is performed over all pure-state convex decompositions of \( \rho \) into \( \rho = \sum_i p_i \ket{\psi_i} \langle \psi_i | \). In other words, in every such decomposition at least one state has nonclassical rank \( R_N(\ket{\psi_i}) \geq N_N(\rho) \), and there exists a decomposition where all pure states have nonclassical rank \( R_N(\ket{\psi_i}) \leq N_N(\rho) \).

Killoran et al [15] showed that there always exists an isometry, consisting of adding an ancilla and applying a global unitary, which maps each pure state of nonclassical rank \( k \) into a bipartite entangled pure state of Schmidt rank \( k \). In fact, as we show below, this result can be straightforwardly extended to the general case of mixed states:

Proposition 1. Let \( \mathcal{H} \) be a \( d \)-dimensional Hilbert space, \( \mathcal{D}(\mathcal{H}) \) the corresponding set of density operators, and \( \mathcal{H}_{\text{anc}} \cong \mathcal{H} \) the Hilbert space of an ancillary system. Then if the classical pure states \( \{ \ket{\chi_i} \} \) form a linearly independent set spanning \( \mathcal{H} \), there exists an isometry \( W : \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}_{\text{anc}} \) such that for any state \( \rho \in \mathcal{D}(\mathcal{H}) \) we have \( N_N(\rho) = N_N(W\rho W^\dagger) \).
Proof. To begin, let us note the fact that the set of all possible pure states belonging to pure-state decompositions of \(\rho \in \mathcal{D}(\mathcal{H})\) is given precisely by the set of pure states in the support of \(\rho\) [40, 41]. By the result of [15], we have that there exists a unitary \(U\) such that \(R_N(|\psi\rangle) = R_N(U(|\psi\rangle \otimes |\psi\rangle_\text{anc})\) \(\forall |\psi\rangle \in \mathcal{H}\) where \(|\psi\rangle_\text{anc} \in \mathcal{H}_\text{anc}\) is a fixed reference state for the ancilla system. The isometry \(W\) is given by attaching the ancilla state \(|\psi\rangle_\text{anc}\) composed with the action of the unitary \(U\). Following [20, 42], we note that there is a one-to-one correspondence between the pure-state decompositions of \(\rho\) and the decompositions of \(\rho' = W \rho W^\dagger\), given exactly by the action of \(W\). Notice in particular that \(W\) can be inverted on its image, and that any \(|\psi\rangle\) in the support of \(\rho'\) has as pre-image \(W^\dagger |\psi\rangle\) in the support of \(\rho\), which means that by the properties of \(W\) one has \(R_N(W^\dagger |\psi\rangle) = R_N(|\psi\rangle)\). Assuming \(\rho\) has \(N_S(\rho) = k\), then it is possible to find a pure-state decomposition of it which only contains states with nonclassicality rank less or equal to \(k\). The pure states in one such decomposition will then be transformed by the action of \(W\) into entangled states of Schmidt rank at most \(k\), which will form a pure-state decomposition of \(\rho'\). This proves that \(N_S(\rho') \leq N_S(\rho)\). On the other hand, suppose \(N_S(\rho') = l\); then it is possible to find a pure-state decomposition of \(\rho'\) such that it only contains states with Schmidt rank less or equal to \(l\). Under the action of \(W\), such a decomposition gives rise to a pure-state decomposition of \(\rho\) whose elements have nonclassicality rank at most \(l\). This proves that \(N_S(\rho) \leq N_S(\rho')\).

In this paper, we show that an analogous faithful conversion of multilevel nonclassicality into genuine multipartite entanglement is always possible. Following [43], we define a pure state \(|\psi\rangle\) to be \(k\)-producible if it can be written as \(|\psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_m\rangle\) with each \(|\psi_i\rangle\) pertaining to at most \(k\) parties, and a mixed state \(\rho\) to be \(k\)-producible if it can be written as a convex combination of \(k\)-producible pure states. We call a state \(\rho\) genuinely \(k\)-partite entangled if it is \(k\)-producible but not \(k-1\)-producible; equivalently, under such conditions we say that \(\rho\) has entanglement depth \(D_E(\rho) = k\) [44]. A 1-producible state \(\rho\) has \(D_E(\rho) = 1\) and is fully separable.

Theorem 2. Let \(\mathcal{H}\) be a \(d\)-dimensional Hilbert space, and \(\mathcal{H}_\text{anc}\) the Hilbert space of an ancillary system. Then if the classical pure states \(\{|c_i\rangle\}_{i=1}^d\in \mathcal{H}\) form a linearly independent set spanning \(\mathcal{H}\), there exists an isometry \(V: \mathcal{H} \rightarrow \mathcal{H} \otimes \mathcal{H}_\text{anc}\) such that for any state \(\rho \in \mathcal{D}(\mathcal{H})\) with nonclassical number \(N_S(\rho) = k\), \(V \rho V^\dagger\) is genuinely \(k+1\)-partite entangled iff \(\rho\) is nonclassical \((2 \leq k \leq d)\) and \(V \rho V^\dagger\) is fully separable iff \(\rho\) is classical \((k = 1)\).

Proof. We adapt the methods of [15] to show the existence of this mapping. Let us consider the case of pure states first. Define

\[ |c_i\rangle = |\chi_i\rangle \otimes |\psi_\text{anc}\rangle \in \mathcal{H} \otimes \mathcal{H}_\text{anc}^{\otimes d} \]  

with \(|\psi_\text{anc}\rangle \in \mathcal{H}_\text{anc}^{\otimes d}\) a fixed (fully unentangled) reference state of the ancilla systems. Define \(\{|b_i\rangle\}_{i=1}^d\in \mathcal{H}_\text{anc}^{\otimes d}\) as

\[ |b_i\rangle = |0\rangle^{i-1} \otimes |\lambda\rangle \otimes |0\rangle^{d-i} \]  

with \(|\lambda\rangle = \sqrt{\lambda}|0\rangle + \sqrt{1-\lambda}|1\rangle\), where \(|0\rangle, |1\rangle \in \mathcal{H}_\text{anc}\) are orthonormal, and \(0 \leq \lambda \leq 1\). Recall that the Gram matrix of a set of states \(\{|\phi_i\rangle\}\) is defined as \([G^{\otimes d}]_{ij} = \langle \phi_i | \phi_j \rangle\), and has full rank iff the \(|\phi_i\rangle\)'s are linearly independent [45]. Define a \(\mu\)-dependent matrix \(B(\mu)\) such that \([B(\mu)]_{ij} = 1\) if \(i = j, \mu\) if \(i \neq j\). We have \(G^{\mu} = B(\mu)\). Define \(M(\epsilon) = G^{\mu} \circ B(1 + \epsilon)\) where \(\circ\) is the Hadamard (that is, entrywise) product. Since \(\lim_{\epsilon \rightarrow -\infty} M(\epsilon) = G^{\mu} > 0\) and \(\text{diag}(M(\epsilon)) = (1, 1, \ldots, 1)\), it follows that, for sufficiently small \(\epsilon > 0\), \(M(\epsilon)\) is the Gram matrix \(G^{\mu}\) of a set of linearly independent states \(\{|a_i\rangle\}_{i=1}^d\). We then have \(G^{(\epsilon)} = G^{\mu} \circ B\left(\frac{1}{\epsilon + 1}\right) = G^{\mu} \circ G^{\mu}, \) for \(\lambda = (1 + \epsilon)^{-1}\), which means that the sets of states \(\{|c_i\rangle\}\) and \(\{|a_i\rangle \otimes |b_i\rangle\}\) have equal Gram matrices, and so there exists a unitary \(U\) such that \(U|c_i\rangle = |a_i\rangle \otimes |b_i\rangle \forall i\) [45, 46]. The isometry \(V\) is defined by the composition of attaching the ancilla state \(|\psi_\text{anc}\rangle\) following the action of \(U\).

Now consider a general pure qudit state \(|\psi\rangle = \sum_{i=1}^d \psi_i|\chi_i\rangle\). Then,

\[ |\psi'\rangle = V|\psi\rangle = \sum_{i=1}^d \psi_i|a_i\rangle |b_i\rangle = \sum_{i=1}^d \psi_i|a_i\rangle |0\rangle^{i-1} |\lambda\rangle |0\rangle^{d-i}. \]

(3)

It is convenient to use the fact that the entanglement depth of \(|\psi'\rangle\) is not affected by a local filter \(S \otimes I^{\otimes d}\), with \(S\) a qudit operator such that \(S|\lambda\rangle = |\lambda\rangle\), and \(L\) a qudit operator such that \(L|0\rangle = |0\rangle, L|1\rangle = |1\rangle\). Thus, we can study the entanglement depth of the state

\[ |\tilde{\psi}'\rangle \propto \sum_{i=1}^d \psi_i|\tilde{b}_i\rangle |0\rangle^{i-1} |1\rangle |0\rangle^{d-i} = \sum_{i=1}^d \psi_i|\tilde{b}_i\rangle |2^{d-i} \}

(4)

where \(|2^{d-i}\rangle\) is the string of qubits corresponding to \(2^{d-i}\) in binary (padded with zeros from the left as needed), e.g. \(|2^1\rangle = |00 \cdots 01000\rangle\) since \(2^1 = 1000_2\). It is evident that \(|\tilde{\psi}'\rangle\) is fully product iff there is only one term in the
superposition, that is, \( R_N(\{|\psi\rangle\}) = 1 \) iff \( D_k(\{|\psi\rangle\}) = 1 \). In the following we will consider \( R_N(\{|\psi\rangle\}) \geq 2 \), and in this case we will prove that \( D_k(\{|\psi\rangle\}) = R_N(\{|\psi\rangle\}) + 1 \).

To show that \( R_N(\{|\psi\rangle\}) = k \geq 2 \) implies \( D_k(\{|\psi\rangle\}) = k + 1 \), assume w.l.o.g. that the \( k \) nonzero coefficients \( c_i \) are the first ones. Then \( \{|\psi\rangle\} = \sum_{i=1}^{k} c_i |i\rangle |0\rangle^{d-k} \), and the claim follows by showing that \( \sum_{i=1}^{k} c_i |i\rangle |0\rangle^{d-k} = |1\rangle |0\rangle^{d-k} \) cannot be factorized in any nontrivial way. This holds, as the reduced state of the \( k \) ancillary qubits is proportional to \( \sum_{i=1}^{k} c_i |i\rangle |0\rangle^{d-k} \otimes |1\rangle \otimes |0\rangle^{d-k} \), so the marginal state of any subset of these \( k \) qubits is evidently mixed. On the other hand, to prove that \( D_k(\{|\psi\rangle\}) = D_k(V|\psi\rangle) = k + 1 \geq 3 \) implies \( R_N(\{|\psi\rangle\}) = k \), notice that the isometry is invertible on its image. Thus, \( |\psi\rangle = V^{\dagger}|\psi\rangle \); since we have just proven that \( D_k(V|\psi\rangle) = R_N(\{|\psi\rangle\}) + 1 \), we arrive at the claim for pure states.

The mixed-state case follows [20, 42] by noting that there is a one-to-one correspondence between the pure state decompositions \( \{|\psi\rangle, |\psi'\rangle\} \) of \( \rho = \sum_{i=1}^{m} f_i |\psi_i\rangle \otimes |\psi'_i\rangle \) of each input–output pair of states respecting the relation just discussed: either \( R_N(\{|\psi\rangle\}) = D_k(\{|\psi\rangle\}) = 1 \) or \( R_N(\{|\psi\rangle\}) = D_k(\{|\psi\rangle\}) = 1 \). Indeed, the pure-state mapping with the above properties, together with the definitions of nonclassical number and entanglement depth, entail that \( N_N(\rho) = m \) implies \( D_k(\rho') \leq m + 1 \), and, in turn, \( D_k(\rho') = 1 \implies N_N(\rho') \leq l - 1 \). These relations can only be satisfied for \( l = m + 1 \).

Theorem 2 shows that there always exists an isometry which faithfully converts the \( k \)-level nonclassicality of a quantum system into multipartite entanglement in \( k \) other ancillary systems. We note that the specifics of the mappings are not fixed by the theorem, and one could always devise other ways to convert the nonclassicality into entanglement. In particular, the mappings presented in the proofs only use two levels of each ancillary system, resulting in entanglement akin to that of W states [47]. One may consider other kinds of operations which create qualitatively different multipartite entanglement—for instance, one can instead attach a number \( d \) of \( d \)-dimensional ancilla systems and choose \( \{|b_i\rangle\}_{i=1}^{d} \) such that \( |b_i\rangle = |\lambda\rangle^{\otimes d} + |\lambda\rangle^{\otimes d} \) where \( \{|j\rangle\} \) is now an orthonormal basis for \( \mathcal{H}_{\text{anc}} \). Following a similar argument to theorem 2, this will then introduce a generalized GHZ-type entanglement between the qudits, entangling as many levels of the systems as the nonclassical rank of the original state. However, the choice of a \( W \)-type mapping in the theorems makes the conversion quite appealing in practice, as it only requires qubit ancillas, and, as we show below, enables one to create entanglement by a sequential application of two-body gates on the nonclassical system and each ancilla.

### 3. Coherence conversion protocol

We will now specialize to the framework of quantum coherence [4, 7, 9, 12]. Here, the classical states \( \{|i\rangle\}_{j=1}^{d} \) are taken to form a fixed orthonormal basis for \( \mathcal{H} \). Analogously to nonclassicality, we can then define a hierarchy of coherence levels by considering the coherence rank \( R_C(\{|\psi\rangle\}) \), defined to be the number of nonzero coefficients \( c_i \) that a state \( |\psi\rangle = \sum_i c_i |i\rangle \) has in this basis [5, 6]. We then define the coherence number

\[
N_C(\rho) = \min_{\{|\psi\rangle\}} \max_{\{p_i, |i\rangle\}} R_C(\{|\psi\rangle\})
\]

for a mixed state \( \rho \) accordingly. We will refer to states with coherence number \( k \) as \( k \)-coherent states. Clearly, \( 1 \)-coherence corresponds to classicality, \( k \)-coherence for any \( k \geq 2 \) stands as a fine graining of the usual notion of coherence, and \( d \)-coherence is the maximal coherence level of a \( d \)-level system.

The \( k \)-coherence of a single qudit can be converted into multipartite entanglement in different physical ways. To show this, we design a protocol to convert \( k \)-coherence into \( k + 1 \)-partite entanglement between the qudit and \( k \) qubit ancillas (following theorem 2), realizable by a sequential application of CNOT gates (see figure 1). We then provide a natural mapping of \( k \)-coherence into \( k \)-body entanglement, which can be accomplished by a second step which disentangles the qudit system—either by unitary transformations as in figure 1(a), or by one-way LOCC as in figure 1(b). The latter scheme realizes an operational scenario in which input agents are constrained to the resource theory of \( k \)-coherence, having at disposal only incoherent ancillas and incoherent operations as used in the first step, while output agents are constrained to the resource theory of entanglement, being bound to use LOCC as in the second step.

We illustrate the scheme for pure states, noting that it extends straightforwardly to mixed states. Let \( |\Psi\rangle = |\psi^d\rangle \otimes |0\rangle^{\otimes d} \) be the state of the composite system consisting of the qudit initialized in \( |\psi^d\rangle \) and \( d \) ancilla qubits in a reference pure state \( |0\rangle^{\otimes d} \). Consider a unitary activation operation \( U^\text{act} \) which consists of a sequence of generalized CNOT gates \( \mathbf{I}_d - |i\rangle \langle i| \otimes \mathbf{1} + |i\rangle \langle i| \otimes \sigma_x \) with \( \sigma_x \) the Pauli \( x \) matrix, between the qudit and the \( i \)-th ancillary qubit. Explicitly, the sequence realizes the unitary

\[
U^\text{act} = \prod_{i=1}^{d} (\mathbf{I}_d - |i\rangle \langle i| \otimes \mathbf{1} + |i\rangle \langle i| \otimes \sigma_x)
\]
Figure 1. Schemes of two protocols to convert $k$-coherence into multipartite entanglement. Both protocols begin with the global unitary operation $U_A$ which sequentially entangles each level of the qudit system in the state $|\psi^d\rangle$ with a corresponding ancillary qubit by generalized CNOT gates, resulting in a $k + 1$-partite entangled state. One can then decouple the qudit system either (a) by a unitary transformation $U_B$, consisting of a Fourier transform and a disentangling unitary $U_D$, or (b) via a one-way LOCC operation $\Delta$. Both protocols result in genuine $k$-partite entanglement between the ancillary qubits.

$$U_A = \sum_{i=1}^{d} |i\rangle \otimes 1_{d-1}^{\otimes} \otimes \sigma_i \otimes 1_{d-i}^{\otimes},$$

which transforms the state $|\Psi\rangle = \sum_{i=1}^{d} c_i |0\rangle^{\otimes d}$ into $|\Psi'\rangle = U_A |\Psi\rangle = \sum_{i=1}^{d} c_i |2^{d-i}\rangle$.

To complete the protocol by mapping into $k$-partite entanglement among the qubit ancillas only, we now give two alternative approaches. Both methods begin by performing a quantum Fourier transform (QFT) $|j\rangle \rightarrow \frac{1}{\sqrt{d}} \sum_{m=1}^{d} e^{2\pi i j m / d} |m\rangle$ on the qudit only. Then, in the first approach (figure 1(a)), we can apply a unitary

$$U_D = \sum_{j,m=1}^{d} e^{-2\pi i j m / d} |m\rangle \langle m| \otimes |2^{d-j}\rangle \langle 2^{d-j}|$$

acting on the $j$th ancillary qubit. After the action of the QFT and $U_D$, which jointly define the global unitary $U_B$, the output will be the product state $U_D |\Psi'\rangle = |\Phi^+\rangle |\Psi''\rangle$, where $|\Phi^+\rangle = \sum_{i=1}^{d} |i\rangle$ is the maximally coherent state of the qudit, and $|\Psi''\rangle = \sum_{i=1}^{d} c_i |2^{d-i}\rangle$ is a $k$-partite entangled state of the qudit ancillas.

An alternative approach (figure 1(b)), which might lend itself to a more efficient implementation as it does not require global interactions, is to realize the decoupling of the qudit by an operation $\Delta$ consisting of one-way LOCC (see e.g. [42]). After performing the QFT, one can measure the qudit in the $|m\rangle$ basis and, depending on the measurement result $m$, apply the local unitary $U_D^{(m)} = |0\rangle \langle 0| + e^{-2\pi i j m / d} |1\rangle \langle 1|$ to the remaining $d$ qubits. We then obtain the final state $\Delta(|\Psi'\rangle) = |\Psi''\rangle$, which is exactly the same as the state of the qudits after the unitary transformation $U_B$ from the previous approach.

We can formalize the properties of the protocol as follows, casting the result in terms of mixed states in general.

**Theorem 3.** Given the above conversion protocol, consisting of the activation unitary $U_A$ and the decoupling operation (either via $U_B$ or $\Delta$), with $\rho' = U_A (\rho \otimes |0\rangle \langle 0|^{\otimes d}) U_A^\dagger$ and $\rho'' = \Delta(\rho')$, the following statements are equivalent for $2 \leq k \leq d$:

(i) $N_C(\rho) = k$;

(ii) $D_{k+1}(\rho') = k + 1$;

(iii) $D_k(\rho'') = k$.

**Proof.** The equivalence between (i) and (ii) is a direct application of theorem 2. To prove that (i) implies (iii), we first consider pure states, and assume w.l.o.g. that the $k$ nonzero coefficients are the first ones. Then the last $d - k$ qubits in $|\Psi''\rangle$ are in the initial product state $|0\rangle^{\otimes d-k}$, and we need to prove that the first $k$ qubits are genuinely multipartite entangled. This is the case since any nontrivial subset of such qubits is mixed. That (iii)
implies (i) can then be proven by observing, as in the proof of theorem 2, that the isometry from \( |\psi^D\rangle \) to \( |\Psi^D\rangle \) can be inverted, and using the just proven fact that (i) implies (ii). The extension to mixed states follows the exact same steps as in theorem 2.

We notice that (i) and (iii) are actually also equivalent for \( k = 1 \), which does not hold in the case of (i) and (ii) since classicality does not lead to entanglement creation.

4. Quantitative relations

In any resource theory, one can define a faithful class of quantifiers by considering the distance to the set of nonresource states [14, 48, 49]. In the cases of bipartite entanglement and standard coherence (i.e., 2-coherence in our framework), the corresponding nonresource sets are the sets of separable states \( \mathcal{S} \) and incoherent states \( \mathcal{I} \), respectively [7, 50]. For the case of \( k \)-partite entanglement, one can define the nonresource set as the set of \( k - 1 \)-producible states \( \mathcal{P}^{(k-1)} \) [43], i.e., states which are at most \( k - 1 \)-partite entangled. Similarly for \( k \)-coherence, we consider the set \( \mathcal{C}^{(k-1)} \) of states which are at most \( k - 1 \)-coherent. We then define the distance-based quantifiers as follows.

**Definition 4.** Given a quasi-metric \( D(\rho, \sigma) \) contractive under CPTP maps, we define the distance-based measure of \( k \)-partite entanglement as

\[
E_D^{(k)}(\rho) = \inf_{\varsigma \in \mathcal{P}^{(k-1)}} D(\rho, \varsigma)
\]  

and the distance-based measure of \( k \)-coherence as

\[
C_D^{(k)}(\rho) = \inf_{\sigma \in \mathcal{C}^{(k-1)}} D(\rho, \sigma).
\]

The distance-based quantifiers of \( k \)-coherence and \( k \)-partite entanglement have many useful properties which allow us to relate the two resource quantitatively. In particular, within the distance-based framework, we prove the following relation between the degree of coherence of a state \( \rho \) and the multipartite entanglement of the output states \( \rho' = U_A (\rho \otimes |0\rangle \langle 0|) U_A^\dagger \) and \( \rho'' = \Delta(\rho') \) obtained from the conversion protocol of theorem 3:

**Theorem 5.** Let \( D \) be any distance contractive under CPTP maps. Then

\[
C_D^{(k)}(\rho) \geq E_D^{(k+1)}(\rho'),
\]

\[
C_D^{(k)}(\rho) \geq E_D^{(k)}(\rho'').
\]

**Proof.** Let \( \mathcal{P}^{(k)} \) denote the subset of \( \mathcal{P}^{(k)} \) spanned by states of the form \( |\Psi^D\rangle = \sum_{i=1}^d c_i |2d-i\rangle \) as obtained from the first step of the conversion protocol in theorem 3. Similarly, let \( \mathcal{R}^{(k-1)} \) denote the subset of \( \mathcal{P}^{(k-1)} \) spanned by \( |\Psi''\rangle = \sum_{i=1}^d c_i |2d-i\rangle \) as obtained from the second step of the same protocol.

Let us consider \( \rho' \) first. We have that

\[
C_D^{(k)}(\rho) = \inf_{\sigma \in \mathcal{C}^{(k-1)}} D(\rho, \sigma)
\]

\[
= \inf_{\sigma \in \mathcal{C}^{(k-1)}} D(U_A \rho \otimes |0\rangle \langle 0| U_A^\dagger , U_A \sigma \otimes |0\rangle \langle 0| U_A^\dagger )
\]

\[
= \inf_{\sigma \in \mathcal{C}^{(k-1)}} D(\rho', U_A \sigma \otimes |0\rangle \langle 0| U_A^\dagger )
\]

\[
= \inf_{\delta \in \mathcal{B}^{(k)}} D(\rho', \delta)
\]

\[
\geq \inf_{\varsigma \in \mathcal{P}^{(k)}} D(\rho', \varsigma)
\]

\[
= E_D^{(k+1)}(\rho'),
\]

where we have used theorem 3, as well as the facts that \( D(\rho \otimes \tau, \sigma \otimes \tau) = D(\rho, \sigma) \) and \( D(U\rho U^\dagger, U\sigma U^\dagger) = D(\rho, \sigma) \) for any contractive distance \( D \). Equality clearly holds when there exists \( \delta \in \mathcal{B}^{(k)} \) such that

\[
\inf_{\varsigma \in \mathcal{P}^{(k)}} D(\rho', \varsigma) = D(\rho', \delta).
\]

An analogous argument holds for \( \rho'' \). One can either follow the steps above with the unitary transformation \( U_{\delta} \) or note the contractivity of the distance \( D \) under the LOCC operation \( \Delta \) and obtain:
The amount of $k$-coherence present in the initial state thus places quantitative constraints on the multipartite entanglement one can obtain from it.

We can obtain a particularly interesting family of distance-based quantifiers by setting $D(\rho, \sigma) = 1 - F(\rho, \sigma)$, with

$$F(\rho, \sigma) = \text{Tr} \left( \sqrt{\rho \sigma} \sqrt{\rho \sigma} \right)^2$$

being the (squared) fidelity [51, 52]. These quantifiers are related to the family of geometric measures of $k$-coherence $C_{G}^{(k)}$ and $k$-partite entanglement $E_{G}^{(k)}$, which directly generalize their counterparts defined first for entanglement [34, 35] and standard quantum coherence [7, 26]:

**Definition 6.** The geometric measure of $k$-partite entanglement is given by

$$E_{G}^{(k)}(\psi) = \inf_{|\psi\rangle \in \mathcal{P}^{k-1}} (1 - F(|\psi\rangle, |\psi\rangle))$$

and similarly for the geometric measure of $k$-coherence:

$$C_{G}^{(k)}(\psi) = \inf_{|\psi\rangle \in \mathcal{P}^{k-1}} (1 - F(|\psi\rangle, |\psi\rangle))$$

where $F(|\psi\rangle, |\psi\rangle) = |\langle \sigma | \psi \rangle|^2$ is the (squared) fidelity.

In fact, the geometric measures and the fidelity-based distance quantifiers can be shown to be equal to each other, as we prove below.

**Proposition 7.** The following relation holds for the geometric measures:

$$E_{G}^{(k)}(\rho) = \inf_{\sigma \in \mathcal{P}^{k-1}} (1 - F(\rho, \sigma))$$

$$C_{G}^{(k)}(\rho) = \inf_{\sigma \in \mathcal{P}^{k-1}} (1 - F(\rho, \sigma)),$$

where $F(\rho, \sigma) = (\text{Tr} \sqrt{\rho \sigma} \sqrt{\rho \sigma})^2$ is the (squared) fidelity.

**Proof.** Let $X$ denote either $\mathcal{P}^{(k-1)}$ or $\mathcal{C}^{(k-1)}$. We know that $X$ is a closed convex set with its extremal points $\text{ext}(X)$ given by pure states, so by the result of theorem 2 in the appendix of [35] we have

$$\max_{\sigma \in X} F(\rho, \sigma) = \max_{\{p_{i}, \rho_{i}\}} \sum_{i} p_{i} \max_{|\psi\rangle \in \text{ext}(X)} F(\rho_{i}, |\psi\rangle) \langle \psi | \rangle$$

where the maximization is performed over all convex mixed-state decompositions of $\rho = \sum_{i} p_{i} \rho_{i}$. Let $\{p_{i}, \rho_{i}\}$ be the decomposition which realizes the first maximization on the right-hand side, and note that every such $\rho_{i}$ can in turn be expressed as a convex decomposition into pure states $|\psi_{i}\rangle$ as $\rho_{i} = \sum_{j} d_{ij} |\psi_{j}\rangle \langle \psi_{j} |$. Let $\{|\psi_{j}\rangle\}$ be the states which realize the second maximization for each $\rho_{i}$. We then get
\[
\max_{\sigma \in \mathcal{X}} F(\rho, \sigma) = \sum_i p_i \max_{|\delta| \in \text{ext}(X)} F(\rho_i, |\delta\rangle \langle \delta|) \\
= \sum_i p_i F(\rho_i, |\delta\rangle \langle \delta|) \\
= \sum_{i,j} p_i q_j^* \langle \delta_i | \psi_j \rangle \langle \psi_j | \delta_i \rangle
\]
which shows that the maximum in equation (18) is in fact always reached by a pure-state decomposition of \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \).

Remarkably, under the geometric quantifiers, the \( k\)-coherence of any state and the converted \( k + 1\)-partite entanglement are in fact equal. The result relies on the following lemma, which shows that for any pure state \( |\psi'\rangle \) obtained from the conversion protocol, it suffices to optimize the distance-based quantifier of \( k + 1\)-partite entanglement over the set of \( k\)-producible output states of the protocol, instead of the whole set of \( k\)-producible states.

**Lemma 8.** Given a state of the form
\[
|\psi\rangle = \sum_{i=1}^d c_i |i\rangle |2^{d-i}\rangle,
\]
where we can take \( |c_1| \geq |c_2| \geq \ldots \geq |c_d| \) without loss of generality, the closest \( k\)-producible state with respect to the fidelity-based geometric measure of entanglement can be chosen as a state \( |\psi^*\rangle \in \mathcal{B}^{(k)} \),

In other words, there exists \( |\psi^*\rangle \in \mathcal{B}^{(k)} \) such that
\[
\max_{|\sigma| \in \mathcal{P}^{(k)}} F(|\psi\rangle, |\sigma\rangle) = \max_{|\sigma| \in \mathcal{B}^{(k)}} F(|\psi\rangle, |\sigma\rangle) = F(|\psi\rangle, |\psi^*\rangle).
\]

**Proof.** Recall that, by theorem 1, a state in \( \mathcal{B}^{(k)} \) has \( p \) nonzero coefficients (\( 2 \leq p \leq d \)) iff it is \( p + 1\)-partite entangled. Therefore, we have that any \( |\omega\rangle \in \mathcal{B}^{(k)} \) is given by
\[
|\omega\rangle = \sum_{j \in J} d_j |j\rangle |2^{d-j}\rangle,
\]
where \( J \) is a subset of at most \( k - 1 \) elements of \( \{1, \ldots, d\} \). Hence
\[
F(|\psi\rangle, |\omega\rangle) = |\langle\psi|\omega\rangle|^2 \\
= \left| \sum_{i,j \in J} c_i d_j \langle i | j \rangle \langle 2^{d-i} | 2^{d-j}\rangle \right|^2 \\
= \left| \sum_{j \in J} c_j d_j \right|^2 \\
\leq \sum_{j \in J} |c_j|^2 \sum_{j \in J} |d_j|^2 \\
= \sum_{j \in J} |c_j|^2 \\
\leq \sum_{i=1}^{k-1} |c_i|^2
\]
using the Cauchy–Schwarz inequality and the fact that the coefficients \( |c_i| \) are arranged in nonincreasing order, so the choice of the first \( k - 1 \) coefficients maximizes the expression. This bound is saturated by the renormalised state given by
\[
|\psi^*\rangle = \frac{\sum_{i=1}^{k-1} c_i |i\rangle |2^{d-i}\rangle}{\sqrt{\sum_{j=1}^{k-1} |c_j|^2}} \in \mathcal{B}^{(k)}
\]
and so it is tight.

Therefore, we need to show that for any \( |\phi\rangle \in \mathcal{P}^{(k)} \) we have \( |\langle\psi|\phi\rangle|^2 \leq \sum_{j=1}^{k-1} |c_j|^2 \).

For a general \( k\)-producible state, we have to consider several different cases corresponding to different partitions. Consider a general \( k\)-producible state \( |\psi^{(m)}\rangle \), where the qudit is entangled with \( n \) qubits and the remaining \( (d - n) \) qubits are in some arrangement—we do not explicitly assume anything about the state of the \( (d - n) \) qubits. The state has the following form:
\[ |\phi^{(n)}\rangle = |\text{qudit} + n \text{ qubits}\rangle \otimes |d - n \text{ qubits}\rangle \]
\[ = |\phi_A^{(n)}\rangle \otimes |\phi_B^{(n)}\rangle. \]

We necessarily have that \( n \leq k - 1 \), because otherwise \( |\phi^{(n)}\rangle \) would not be \( k \)-producible.

Note that for a general bipartite state \(|\rho_{AB}\rangle\), it follows from the Schmidt decomposition that \([34, 53]\)
\[
\max_{\text{separable} \ |\rho_{AB}\rangle} \langle \eta_{AB} | \rho_{AB} \rangle F = \lambda_{\text{max}} \left( \mathrm{Tr}_A( |\rho_{AB} \rangle \langle \rho_{AB} |) \right),
\]
where \( \lambda_{\text{max}} \) denotes the largest eigenvalue. In our case, we can treat \( k \)-partite\end{vig}
\[ \text{extension of} \ |\phi^{(n)}\rangle \text{as required.} \]

Given \(|\phi^{(n)}\rangle\), we can treat \(|\psi\rangle\) as a bipartite state where the subsystem \( A \) is comprised of the qudit and \( n \) qubits, and \(|\phi^{(n)}\rangle\) is the corresponding product state. We then have
\[
\mathrm{Tr}_{\text{qudit}}( |\psi\rangle \langle \psi| ) = \sum_{i,j,m=1}^d c_i \sigma_i \langle m | j \rangle \langle j | m \rangle |2^{d-i}| \langle 2^{d-j}| = \rho_f,
\]
\[
\mathrm{Tr}_{\text{leftmost qubits}}( \rho_f ) = \sum_{j=1}^n |c_j|^2 |00 \ldots 0\rangle \langle 00 \ldots 0| + \sum_{j=n+1}^d |c_j|^2 |2^{d-j}| \langle d-n , 2^{d-j}| = \rho^{(n)}_f,
\]
where we have introduced a subscript in the notation \( |2^{d-j}|_{d-n} \) to indicate that there are \( d - n \) qubits left over. Notice that the only possible nonzero eigenvalues of \( \rho^{(n)}_f \) are given by: \( \sum_{j=1}^n |c_j|^2, |c_{n+1}|^2, |c_{n+2}|^2, \ldots, |c_d|^2 \). Since the coefficients \( |c_i| \) are arranged in nonincreasing order by assumption, it follows that
\[
\max_{|\phi^{(n)}\rangle \in \mathcal{D}^k} \langle \phi^{(n)} | \psi \rangle \|^2 \leq \lambda_{\text{max}}( \rho^{(n)}_f ) = \sum_{i=1}^n |c_i|^2 \leq \sum_{j=1}^{k-1} |c_j|^2
\]
as required.

The above lemma finally allows us to prove the equality between the geometric quantifiers for \( k \)-coherence and \( k + 1 \)-partite entanglement in the first step of the conversion protocol, which is the last main result of this paper.

**Theorem 9.** Given \( \rho \) and the transformed state \( \rho' \) as described in the conversion protocol, we have
\[
C_{G}^{(k)}(\rho) = E_{G}^{(k+1)}(\rho').
\]

**Proof.** The proof follows the methods of \([26, 35]\).

By theorem 5 and proposition 7, this result amounts to showing that there exists a state \( \chi \in \mathcal{B}^{(k)} \) which is the closest \( k \)-producible state to \( \rho' \) with respect to the distance given by \( D(\rho, \sigma) = 1 - F(\rho, \sigma) \). In other words, we need to find \( \chi \in \mathcal{B}^{(k)} \) such that \( E_{G}^{(k+1)}(\rho') = 1 - F(\rho', \chi) \).

First, let \( \{ P_i, |\phi_i\rangle \} \) be the optimal convex decomposition of \( \rho' \) which realizes the infimum in the convex roof extension of \( E_{G}^{(k+1)} \), that is,
\[
E_{G}^{(k+1)}(\rho') = \sum_i P_i \ E_{G}^{(k+1)}( |\phi_i\rangle \langle \phi_i|).
\]

Define \( \{ |\xi_i\rangle \} \in \mathcal{D}^{(k)} \) to be the closest \( k \)-producible states to each of the states \( \{ |\phi_i\rangle \} \) with respect to the fidelity-based distance, that is,
\[
E_{G}^{(k+1)}( |\phi_i\rangle \langle \phi_i| ) = 1 - F( |\xi_i\rangle , |\phi_i\rangle ) \quad \forall i.
\]

Now, notice that the support of \( \rho' \) is spanned by states of the form
\[
|\psi'\rangle = \sum_i P_i |i\rangle |2^{d-i}\rangle \quad \in \mathcal{B}^{(k)},
\]
which means that any pure state in a convex decomposition of \( \rho' \) can be expressed as a complex linear combination of such \( |\psi'\rangle \). In particular, each of the states \( \{ |\phi_i\rangle \} \) can be written as
\[
|\phi_i\rangle = \sum_j r_{ij} |j\rangle |2^{d-j}\rangle.
\]
By lemma 8, the closest $k$-producible state to each $|\phi_j\rangle$ is a state $|\xi_j\rangle \in \mathcal{B}^{(k)}$, and so we have
\begin{equation}
|\xi_j\rangle = \sum_{i=1}^{k-1} c_i |j,j\rangle |2^{d-j}\rangle.
\end{equation}

Now, define
\begin{equation}
\chi = \sum_j q_j |\xi_j\rangle \langle \xi_j|
\end{equation}
with coefficients
\begin{equation}
q_j = p_j \frac{1 - E_G^{(k+1)}(|\phi_j\rangle)}{1 - E_G^{(k+1)}(\rho')}.
\end{equation}
Since each $|\xi_j\rangle$ is in $\mathcal{B}^{(k)}$, we get that $\chi \in \mathcal{B}^{(k)}$. Recalling that $\sqrt{F}$ satisfies the so-called strong joint concavity property \cite{38}, defined as
\begin{equation}
\sqrt{F} \left( \sum_i a_i |\alpha_i\rangle \langle \alpha_i| + \sum_i b_i |\beta_i\rangle \langle \beta_i| \right) \geq \sum_i \sqrt{a_i b_i} F(|\alpha_i\rangle, |\beta_i\rangle),
\end{equation}
we get
\begin{equation}
\sqrt{F}(\rho', \chi) \geq \sum_j p_j q_j \sqrt{F(|\phi_j\rangle, |\xi_j\rangle)} = \sum_j p_j^2 \frac{F(|\phi_j\rangle, |\xi_j\rangle)^2}{1 - E_G^{(k+1)}(\rho')} = \sqrt{1 - E_G^{(k+1)}(\rho')}
\end{equation}
which follows by equations (31) and (30). This gives
\begin{equation}
E_G^{(k+1)}(\rho') \geq 1 - F(\rho', \chi)
\end{equation}
and since $\chi \in \mathcal{P}^{(k)}$ is a convex combination of $k$-producible pure states, by proposition 7 we also have
\begin{equation}
E_G^{(k+1)}(\rho') \leq 1 - F(\rho', \chi)
\end{equation}
and so $\chi$ is the closest $k$-producible state to $\rho'$. But since $\chi \in \mathcal{B}^{(k)}$ by construction, theorem 5 gives
\begin{equation}
C_G^{(k)}(\rho) = E_G^{(k+1)}(\rho')
\end{equation}
as required. \hfill \Box

The above result has implications for the quantification of $k + 1$-partite entanglement, since for any state of the form $\rho'$ as obtained from the conversion protocol in theorem 3, the entanglement can be quantified by considering the quantification of $k$-coherence instead. It has been recently shown that optimization over sets of $k$-coherent states can be expressed as efficiently computable semidefinite programs (SDPs) \cite{54}, and together with the fact that the computation of the fidelity function can be cast as an SDP as well \cite{55, 56}, we have that the geometric measure of $k + 1$-partite entanglement of any state $\rho'$ can be quantified by the following SDP:
\begin{equation}
\sqrt{1 - E_G^{(k+1)}(\rho')} = \max \text{ ReTr}(X)
\text{s.t. } \begin{cases}
\rho' \sum_{I \in \mathcal{J}_{k-1}} X = 0 \\
X = 0 & \forall I \in \mathcal{J}_{k-1} \\
\text{Tr} \left( \sum_{I \in \mathcal{J}_{k-1}} P_I Y_I P_I \right) = 1 \\
Y_I \geq 0 & \forall I \in \mathcal{J}_{k-1} \\
X \in \mathbb{C}^{d \times d},
\end{cases}
\end{equation}
where $\mathcal{J}_{k-1}$ denotes the set of all $k$-element combinations from $\{1, 2, \ldots, d\}$ and $P_I$ denotes the orthogonal projection $P_I = \sum_{i \in I} |i\rangle \langle i|$ \cite{54}.
Moreover, in a very similar way to the proof of lemma 8, one can derive a closed formula for $C_G^{(k)}$ of arbitrary pure states $|\psi\rangle$ as
where $c_i^1$ denotes the $i$th largest coefficient (by absolute value) of $\ket{\psi}$. This entails a closed formula for $E_G^{(k+1)}$ of the corresponding states $\ket{\Psi^i}$ at the output of the conversion protocol. For completeness, we present a full proof of this fact in the appendix.

We note that quantitative relations can also be obtained for other measures of coherence and entanglement based on the convex roof, similarly to the cases in [9, 26, 57, 58]. Such monotones are built by taking suitable functions defined on pure states [59, 60] and extending them to mixed states by minimizing over all pure-state decompositions [61]. Since the conversion of $k$-coherence into multipartite entanglement is isometric, there is a one-to-one correspondence between such decompositions for input and output states, and close relations between equivalent measures can be derived [62].

5. Conclusions

We have investigated the relation between the nonclassicality (in the form of superposition) of a single quantum system and the genuine multipartite entanglement which can be obtained from it in physical processes. We have shown that a faithful conversion of multilevel nonclassicality into multipartite entanglement is always possible by mapping superpositions between $k$ levels of a system into entanglement between the system and $k$ ancillas via unitary operations. As an explicit implementation of this result, we presented a reversible protocol for the conversion of $k$-coherence into genuine multipartite entanglement, showing that the strength of the final entanglement among all parties is bounded by the initial amount of quantum coherence, and can in fact be exactly equivalent under a suitable choice of geometric quantifiers.

This reveals a qualitative and quantitative connection between multilevel nonclassicality and multipartite entanglement, generalizing previous results in the resource theory of quantum coherence [7, 12, 26], and further contributing towards the formalization of nonclassicality as a resource [15, 16, 31, 32, 63]. In particular, multilevel coherence and multipartite entanglement provide significant operational advantages over the resources of standard quantum coherence and bipartite entanglement [13, 54, 64] and are key ingredients for practical applications such as quantum computation, quantum networks, sensing, and metrology [64–67]. By providing constructive schemes for their interchange in compliance with the respective resource theories, our work lays the foundation for a complete characterization of the interrelations between the two fundamental resources, and may further serve as an inspiration for novel hybrid approaches to quantum technologies.

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Note. During completion of this work, an independent investigation of $k$-coherence and its relation to bipartite entanglement of Schmidt rank $k$ was presented by S Chin [58, 68].

Appendix

Proposition 10. Given an orthonormal basis $\{\ket{i}\}$, for any pure state $\ket{\psi} = \sum c_i \ket{i}$ it holds that

$$C_G^{(k)}(\ket{\psi}) = 1 - \sum_{i=1}^{k-1} |c_i|^2,$$

where $c_i^1$ denotes the $i$th largest coefficient (by absolute value) of $\ket{\psi}$.

Proof. A general state $\ket{\eta} \in C^{(k-1)}$ is given by

$$\ket{\eta} = \sum_{j \in \mathbb{Z}} d_j \ket{j},$$

where $d_j$ are complex coefficients.
where $I$ is a subset of $k - 1$ elements of the indices $\{1, \ldots, d\}$. Hence
\[
F(|\psi\rangle, |\eta\rangle) = |\langle \psi | \eta \rangle|^2 \\
= \left| \sum_{i=1}^{d} \sum_{j \in I} c_i^* d_j \langle i | j \rangle \right|^2 \\
= \left| \sum_{j \in I} d_j \right|^2 \\
\leq \sum_{j \in I} |c_j|^2 \sum_{i \in I} |d_i|^2 \\
= \sum_{j \in I} |c_j|^2 \\
\leq \sum_{i=1}^{k-1} |c_i|^2
\] (A3)

using the Cauchy–Schwarz inequality and the fact that the choice of $k - 1$ largest coefficients $|c_i|$ maximizes the expression. The bound is tight, since one can always reach it by considering the state
\[
|\psi^{\ast}\rangle = \frac{\sum_{i=1}^{k-1} c_i^* |i\rangle}{\sqrt{\sum_{i=1}^{k-1} |c_i|^2}} \in C^{k-1},
\] (A4)

where $|i\rangle$ are the basis vectors corresponding to the coefficients $c_i^*$ of $|\psi\rangle$. Therefore we have
\[
C^{k-1}_i(|\psi^{\ast}\rangle) = 1 - \sup_{|\eta\rangle \in C^{k-1}} F(|\psi^{\ast}\rangle, |\eta\rangle) = 1 - \sum_{i=1}^{k-1} |c_i|^2.
\] (A5)

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