Approximate and Multipartite Quantum Correlation (Communication) Complexity

Rahul Jain* Zhaohui Wei† Penghui Yao‡ Shengyu Zhang§

Abstract

The concepts of quantum correlation and communication complexity have been proposed to quantify the worst-case computational resources needed in generating bipartite classical distributions or bipartite quantum states in the single-shot setting by Zhang (*Proc. 3rd Innov Theor Comput., pp. 39-59, 2012*). The former characterizes the minimal size of the initial shared state needed if no communication is allowed, and the latter characterizes the minimal amount of communication needed if sharing nothing at the beginning. In this paper, we generalize these two concepts to approximate bipartite cases and various multipartite cases.

1. To generate a bipartite classical distribution $P(x, y)$ approximately, we show that the minimal amount of quantum communication needed can be characterized completely by the approximate PSD-rank of P. This result is obtained based on the fact that the cost to approximate a bipartite quantum state equals that to approximate its exact purifications, which also implies a result for a general bipartite quantum state.
2. In the bipartite case, correlation complexity is always equivalent to communication complexity, but in multipartite cases, this is not true any more. For multipartite pure states, we show that both of them could be characterized by local ranks of subsystems.
3. For any bipartite quantum state, its correlation complexity is always equivalent to that of its optimal purification, while in multipartite cases the former could be smaller strictly than the latter. We characterize the relationship between them by giving upper and lower bounds.
4. For multipartite classical distributions, we show that the approximate correlation complexity could also be characterized by the generalized PSD-rank.

1 Introduction

Shared randomness and quantum entanglement among parties located at different places are important computational resources for various distributed information processing tasks. Thus what is the minimal cost to generate these resources is an important issue, and has attracted a lot of attentions from various aspects [1, 5, 8, 3, 4]. Especially, in [4] the worst-case costs of several single-shot bipartite schemes to generate correlations and quantum entanglement have been characterized, and the specific problems they considered and their results are as follows.

Suppose two parties, Alice and Bob, need to generate random variables X and Y such that (X, Y) is distributed as a target distribution P. If P is not a product distribution, Alice and Bob could generate P

*Department of Computer Science and Centre for Quantum Technologies, National University of Singapore, Singapore. Email: rahul@comp.nus.edu.sg

†School of Physics and Mathematical Sciences, Nanyang Technological University and Centre for Quantum Technologies, Singapore. Email: weizhaohui@gmail.com

‡Centre for Quantum Technologies, National University of Singapore, Singapore. Email: phyao1985@gmail.com

§Department of Computer Science and Engineering and The Institute of Theoretical Computer Science and Communications, The Chinese University of Hong Kong. Email: syzhang@cse.cuhk.edu.hk

by sharing an initial seed distribution (X', Y'), and then performing local operations on it. The minimal size of this seed correlation is defined by *randomized correlation complexity* [3], denoted $R(P)$, where the *size* of a bipartite distribution is defined as the half of the total number of bits. It has been known that $R(P)$ is fully characterized as $\lceil \log_2 \mathtt{rank}_+(P) \rceil$ [3], where $\mathtt{rank}_+(P)$ is the nonnegative rank, a measure in linear algebra with numerous applications in combinatorial optimization [9], nondeterministic communication complexity [10], algebraic complexity theory [11], and many other fields [12]. Meanwhile, if quantum operations are allowed, Alice and Bob could also generate P by replacing the seed distribution by a seed quantum state. In this case, the minimal size of the seed quantum state is defined as *quantum correlation complexity*, denoted $\mathsf{QCorr}(P)$, where the *size* of a bipartite quantum state is the half of the total number of qubits. One of the main results of [4] is that $\mathsf{QCorr}(P)$ could be characterized completely as $\lceil \log_2 \mathtt{rank}_{\mathtt{psd}}^{(2)}(P) \rceil$, where $\mathtt{rank}_{\mathtt{psd}}^{(2)}(P)$ is the PSD-rank of P, a concept recently proposed by Fiorini *et al.* in studies of the minimum size of extended formulations of optimization problems such as TSP [8]. Since $\mathtt{rank}_+(P)$ could be much larger than $\mathtt{rank}_{\mathtt{psd}}^{(2)}(P)$, this shows a huge advantage of quantum schemes over classical ones. Moreover, the targets of quantum schemes could also be any quantum state ρ, and [4] also gave a complete characterization for the cost to generate ρ, denoted $\mathsf{QCorr}(\rho)$. Especially, if ρ is a pure state $|\psi\rangle\langle\psi|$, the approximate $\mathsf{QCorr}(|\psi\rangle\langle\psi|)$ is characterized completely by the Schmidt coefficients of $|\psi\rangle$, closing a possibly exponential gap left in [1].

Actually, Alice and Bob could replace the shared correlations or states discussed above by communication completely. In this case, the minimal amount of communication in classical and quantum schemes are defined by *randomized communication complexity* and *quantum communication complexity* respectively, denoted by $\mathsf{RComm}(P)$ and $\mathsf{QComm}(P)$ or $\mathsf{RComm}(\rho)$ and $\mathsf{QComm}(\rho)$ [3]. For bipartite cases, it turns out that correlation complexity is always equivalent to communication complexity, and this is true for both classical settings and quantum settings [3]. Therefore, in the bipartite case one only needs to discuss one of them.

The concepts of correlation complexity and communication complexity characterized in [4] try to characterize the cost to generate given correlations, and thus it can be said that they reveal some essential properties of target correlations. This might provide us a new insight to understand the complicated mathematical structure of correlations, especially in the quantum case, i.e., quantum entanglement. It is widely known that to figure out the structure of quantum entanglement is a major challenge in quantum information theory. However, in [4] only the bipartite case of these two concepts was considered, and even for this special case, approximate correlation (communication) complexities for general bipartite states or probability distributions have not been characterized either. In this paper, we will generalize correlation complexity and communication complexity to general approximate setting of the bipartite case, and then to multipartite cases. Particularly, we will show that in multipartite cases, these two concepts are fundamentally different, compared with the bipartite case considered in [4]. Our main results are listed as follows.

1.1 Approximate bipartite quantum correlation complexity The approximate version of quantum correlation complexity is naturally defined as follows.

DEFINITION 1. *Let $\epsilon > 0$. Let ρ be a bipartite quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B$. Define*

$$\mathsf{QCorr}_\epsilon(\rho) \stackrel{\text{def}}{=} \min\{\mathsf{QCorr}(\rho') : \rho' \in \mathcal{H}_A \otimes \mathcal{H}_B \text{ and } \mathsf{F}(\rho, \rho') \geq 1 - \epsilon\}$$

For a general bipartite quantum state ρ, since it always holds that $\mathsf{QCorr}(\rho) = \mathsf{QComm}(\rho)$, the results on $\mathsf{QCorr}_\epsilon(\rho)$ are also applicable to approximate quantum communication complexities automatically. Let ρ be in $\mathcal{H}_A \otimes \mathcal{H}_B$, then $\mathsf{QCorr}(\rho)$ is equivalent to the optimal $\mathsf{QCorr}(|\psi\rangle)$, where $|\psi\rangle$ is a purification of ρ in $\mathcal{H}_{A_1} \otimes \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1}$ [4](Throughout the paper, we suppose the subscripts of Hilbert spaces stand for the holders). That is, we have

$$\mathsf{QCorr}_\epsilon(\rho) = \min_{\mathcal{H}_{A_1},\mathcal{H}_{B_1}} \{\lceil \log_2 \texttt{S-rank}(|\psi\rangle)\rceil : |\psi\rangle \text{ is a pure state}$$
$$\text{in } \mathcal{H}_{A_1} \otimes \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1}, \mathsf{F}(\rho, \texttt{tr}_{\mathcal{H}_{A_1}\otimes\mathcal{H}_{B_1}} |\psi\rangle\langle\psi|) \geq 1-\epsilon\}. \tag{1.1}$$

Therefore, the approximate quantum correlation complexity of ρ is determined by the minimal Schmidt rank of its "approximate purification". Here an approximate purification of ρ means a pure state with the reduced density matrix on A and B close to ρ. However, usually the pattern of approximating a mixed state is very complicated, thus the approximate purifications seems not easy to analyze. In the following theorem, however, we will see that this difficulty can be avoided, and approximate correlation complexity can be characterized completely by approximating the *exact* purifications of ρ, and this problem has been well-solved [4].

Lemma 1.1. *Assume that ρ is a quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B$. Let*

$$\mathsf{QCorr}'_\epsilon(\rho) = \min_{\mathcal{H}_{A_1},\mathcal{H}_{B_1}} \{\lceil \log_2 \texttt{S-rank}_\epsilon(|\varphi\rangle)\rceil : |\varphi\rangle \textit{ is a pure state}$$
$$\textit{in } \mathcal{H}_{A_1} \otimes \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1}, \rho = \texttt{tr}_{\mathcal{H}_{A_1}\otimes\mathcal{H}_{B_1}} |\varphi\rangle\langle\varphi|\},$$

then $\mathsf{QCorr}_\epsilon(\rho) = \mathsf{QCorr}'_\epsilon(\rho)$.

Based on Theorem 1.1, we could get the following characterization of $\mathsf{QCorr}_\epsilon(\rho)$ for the special case of ρ being classical. We first define approximate PSD-rank and approximate correlation complexity by classical states as follows.

Definition 2. $P = [p(x,y)]_{x,y}$ *is a bipartite probability distribution, its approximate PSD-rank is*

$$\texttt{rank}^{(2),\epsilon}_{\texttt{psd}}(P) = \min\{\texttt{rank}^{(2)}_{\texttt{psd}}(P') : F(P, P') \geq 1-\epsilon\}. \tag{1.2}$$

where $P' = [p'(x,y)]_{x,y}$ *is another probability distribution.*

Definition 3. *For a bipartite classical state* $\rho = \sum_{x,y} P(x,y)|x\rangle\langle x| \otimes |y\rangle\langle y|$ *in* $\mathcal{H}_A \otimes \mathcal{H}_B\}$*, its quantum correlation complexity by classical state ϵ-approximation is* $\mathsf{QCorr}^{cla}_\epsilon(\rho) = \min\{\mathsf{QCorr}(\rho') : F(\rho,\rho') \geq 1-\epsilon, \rho'$ *is another classical state in* $\mathcal{H}_A \otimes \mathcal{H}_B\}$.

Then the following theorem shows that the most efficient approximate generation of a classical state can always be achieved by another classical state. Moreover, similar with the exact case discussed in [4], the approximate correlation complexity of a classical state could be characterized completely by the approximate PSD-rank.

Theorem 1.1. *For any classical state* $\rho = \sum_{x,y} P(x,y)|x\rangle\langle x| \otimes |y\rangle\langle y|$,

$$\mathsf{QCorr}_\epsilon(\rho) = \mathsf{QCorr}^{cla}_\epsilon(\rho) = \lceil \log_2 \texttt{rank}^{(2),\epsilon}_{\texttt{psd}}(P)\rceil.$$

For the general case, we give the following characterization of $\mathsf{QCorr}_\epsilon(\sigma)$ for an arbitrary quantum state σ.

THEOREM 1.2. *Let σ be an arbitrary quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B$, and $0 < \epsilon < 1$. Let $|x\rangle$, $|x'\rangle$ range over the computational basis states for $\mathcal{H}_A$, and $|y\rangle$, $|y'\rangle$ for $\mathcal{H}_B$. $\{A_x\}$'s and $\{B_y\}$'s are matrices with the same column number l that makes*

$$\sigma = \sum_{x,x';y,y'} |x\rangle\langle x'| \otimes |y\rangle\langle y'| \cdot \mathtt{tr}\Big((A_{x'}^\dagger A_x)^T (B_{y'}^\dagger B_y)\Big). \tag{1.3}$$

For any $0 < \epsilon < 1$, suppose r is the minimum number taken over all possible $\{A_x\}$'s and $\{B_y\}$'s such that for $i \neq j$,

$$\sum_x \langle A_x(i)|A_x(j)\rangle = \sum_y \langle B_y(i)|B_y(j)\rangle = 0, \tag{1.4}$$

and

$$\sum_{i=1}^{r} \Big(\sum_x \langle A_x(i)|A_x(i)\rangle\Big)\Big(\sum_y \langle B_y(i)|B_y(i)\rangle\Big) \geq 1 - \epsilon, \tag{1.5}$$

where for convenience, we denote the i-th column of any matrix A by $|A(i)\rangle$. Then $\mathsf{QCorr}_\epsilon(\sigma) = \lceil \log_2 r \rceil$.

1.2 Multipartite quantum correlation complexity For multipartite cases, it turns out that quantum correlation complexity and quantum communication complexity are not equivalent any more, thus we have to deal with them separately. We first consider the former, which is defined as follows.

DEFINITION 4. *Suppose k parties, A_1, A_2, ..., A_k, share a seed state σ, and ρ is another k-partite quantum state shared by them. Then $\mathsf{QCorr}(\rho)$ is the minimal size of σ such that they can generate ρ by local quantum operations based on σ. We call $\mathsf{QCorr}(\rho)$ the quantum correlation complexity of ρ. Here the size of σ is defined as $\sum_{i=1}^{k} n_i$, where n_i is the number of qubits of σ that are holden by A_i.*

Let us first see the case of pure states. For a bipartite pure state $|\psi\rangle$, Schmidt decompositions help us to characterize $\mathsf{QCorr}(|\psi\rangle)$ and $\mathsf{QComm}(|\psi\rangle)$ perfectly, but multipartite pure states usually do not have such decompositions. It turns out that we have the following theorem.

THEOREM 1.3. *Suppose $|\psi\rangle$ is a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and ρ_A, ρ_B and ρ_C are the reduced density matrices of $|\psi\rangle$ in $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_C$ respectively. Assume*

$$t(|\psi\rangle) = \big\lceil \log_2 r_A \big\rceil + \big\lceil \log_2 r_B \big\rceil + \big\lceil \log_2 r_C \big\rceil,$$

where r_i is the rank of $\rho_i (i = A, B, C)$. Then we have that

$$\mathsf{QCorr}(|\psi\rangle) = t(|\psi\rangle).$$

For an arbitrary bipartite quantum state ρ, it has been mentioned above that $\mathsf{QCorr}(\rho)$ is exactly the minimal $\mathsf{QCorr}(|\psi\rangle)$, where $|\psi\rangle$ is a purification of ρ [4]. Naturally, we may ask, does the same relationship hold for multipartite quantum states? In fact, we will see that this is not the case.

Let ρ be a quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and suppose $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ is an arbitrary purification of ρ. Define

$$\begin{aligned} r(\rho) = \min_{\mathcal{H}_{A_1}, \mathcal{H}_{B_1}, \mathcal{H}_{C_1}} \{&\mathsf{QCorr}(|\psi\rangle) : |\psi\rangle \text{ is a pure state} \\ \text{in } \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}&, \rho = \mathtt{tr}_{\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |\psi\rangle\langle\psi|\}. \end{aligned} \tag{1.6}$$

Then we will prove the following theorem.

THEOREM 1.4. *Assume that ρ is a quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and $r(\rho)$ is defined as in Eq.*(1.6). *Then we have*

$$\mathsf{QCorr}(\rho) \leq r(\rho) \leq \frac{4}{3}\mathsf{QCorr}(\rho).$$

As an example that $r(\rho)$ and $\mathsf{QCorr}(\rho)$ could be different, suppose $\rho_0 = \frac{1}{2}|GHZ\rangle\langle GHZ| + \frac{1}{2}|W\rangle\langle W|$, where $|GHZ\rangle$ and $|W\rangle$ are 3-qubit GHZ state and W state respectively. Apparently, $\mathsf{QCorr}(\rho_0) \leq 3$. On the other hand, we will prove the following result.

LEMMA 1.1. $r(\rho_0) = 4$.

Similar with the bipartite case, we could also consider quantum correlation complexity of multipartite probability distributions. For this purpose, we need to generalize PSD-rank to multipartite cases first.

DEFINITION 5. *Suppose $P = [P(x_1, x_2, ..., x_k)]_{x_1,x_2,...,x_k}$ is a probability distribution on $\mathcal{X}_1 \times \mathcal{X}_2 \times ... \times \mathcal{X}_k$. The psd-rank of P, denoted by $\mathtt{rank}^{(k)}_{\mathtt{psd}}(P)$, is the minimum r such that there are $r \times r$ positive semi-definite matrices C_1, C_2,..., C_k, satisfying that*

$$P(x_1, x_2, ..., x_k) = \sum_{i,j=1}^{r} \prod_{m=1}^{k} C_m(i, j), \tag{1.7}$$

where $C_m(i, j)$ is the (i, j)-th entry of matrix C_m.

For the tripartite case, we have the following theorem.

THEOREM 1.5. *Suppose $P = [P(x, y, z)]_{x,y,z}$ is a probability distribution on $\mathcal{X} \times \mathcal{Y} \times \mathcal{Z}$. Let*

$$\rho = \sum_{x,y,z} P(x, y, z)|x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z|.$$

Then it holds that

$$\frac{3}{4}\left\lceil \log_2 \mathtt{rank}^{(3)}_{\mathtt{psd}}(P)\right\rceil \leq \mathsf{QCorr}(\rho) \leq 3\left\lceil \log_2 \mathtt{rank}^{(3)}_{\mathtt{psd}}(P)\right\rceil.$$

1.3 Multipartite quantum communication complexity

DEFINITION 6. *Suppose k parties, A_1, A_2, ..., A_k, share a quantum state ρ. Then $\mathsf{QComm}(\rho)$ is the minimum number of qubits exchanged between these k parties, initially sharing nothing, to produce ρ at the end of the protocol. We call $\mathsf{QComm}(\rho)$ the quantum communication complexity of ρ.*

Once again, we begin with pure states.

THEOREM 1.6. *Suppose $|\psi\rangle$ is a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and $t(|\psi\rangle)$ is defined as in Theorem 1.3. Then we have that*

$$\frac{1}{2}t(|\psi\rangle) \leq \mathsf{QComm}(|\psi\rangle) \leq \frac{2}{3}t(|\psi\rangle),$$

and both of the two inequalities could be tight.

We now turn to general multipartite quantum states. Interestingly, we will see that for arbitrary multipartite ρ, $\mathsf{QComm}(\rho)$ is always equivalent to the optimal $\mathsf{QComm}(|\psi\rangle)$, where $|\psi\rangle$ is a purification of ρ. As a comparison, we have mentioned above that for quantum correlation complexity, this relationship holds only for the bipartite case.

Theorem 1.7. *Assume that* ρ *is a quantum state in* $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. *Then*

$$\mathsf{QComm}(\rho) = \min_{\mathcal{H}_{A_1},\mathcal{H}_{B_1},\mathcal{H}_{C_1}} \{\mathsf{QComm}(|\psi\rangle) : |\psi\rangle \text{ is a pure state}$$
$$\text{in } \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}, \rho = \mathtt{tr}_{\mathcal{H}_{A_1}\otimes\mathcal{H}_{B_1}\otimes\mathcal{H}_{C_1}} |\psi\rangle\langle\psi|\}.$$

Combining the results in the above two subsections together, we get the following relationship between $\mathsf{QCorr}(\rho)$ and $\mathsf{QComm}(\rho)$ for a general multipartite quantum state ρ.

Theorem 1.8. *Assume that* ρ *is a* k*-partite quantum state in* $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_k$. *Then*

$$\frac{k}{k-1}\mathsf{QComm}(\rho) \le \mathsf{QCorr}(\rho) \le 2\mathsf{QComm}(\rho).$$

1.4 Approximate Quantum Correlation Complexity of Tripartite Pure States With the absence of Schmidt decompositions, it will be challenging to characterize the approximate version of correlation complexity for multipartite pure states. As in [4], in this paper we also consider two different approximations as follows.

Definition 7. *Let* $\epsilon > 0$. *Let* ρ *be a* k*-partite quantum state in* $\mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes ... \otimes \mathcal{H}_{A_k}$. *Define*

$$\mathsf{QCorr}_\epsilon(\rho) \stackrel{\text{def}}{=} \min\{\mathsf{QCorr}(\rho') : \rho' \in \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes ... \otimes \mathcal{H}_{A_k} \text{ and } \mathsf{F}(\rho,\rho') \ge 1-\epsilon\}$$

and

$$\mathsf{QCorr}^{pure}_\epsilon(\rho) \stackrel{\text{def}}{=} \min\{\mathsf{QCorr}(|\phi\rangle) : |\phi\rangle \in \mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes ... \otimes \mathcal{H}_{A_k} \text{ and } \mathsf{F}(\rho, |\phi\rangle\langle\phi|) \ge 1-\epsilon\}.$$

We can see that $\mathsf{QCorr}_\epsilon(\rho)$ *and* $\mathsf{QCorr}^{pure}_\epsilon(\rho)$ *is the complexities of approximating* ρ *by mixed and pure states respectively.*

For simplicity, we only consider the tripartite case, and it could be generalized directly to general cases. Suppose $|\psi\rangle$ is a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. Suppose ρ_A, ρ_B and ρ_C are the reduced density matrices of $|\psi\rangle$ in $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_C$ respectively, and r_A, r_B, r_C are their ranks. We denote the approximate Schmidt rank of $|\psi\rangle$ with respect to the separation (A, BC) as $r_A^{(\epsilon)}$, i.e., $r_A^{(\epsilon)} = \mathtt{S\text{-}rank}_\epsilon^{(A,BC)}(|\psi\rangle)$, similarly for $r_B^{(\epsilon)}$ and $r_C^{(\epsilon)}$, where ϵ is a small positive number. Then we have

Theorem 1.9. *Let* $|\psi\rangle$ *be a pure state in* $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, *and for an arbitrary small positive number* ϵ, *let*

$$t_\epsilon(|\psi\rangle) = \lceil \log_2 r_A^{(\epsilon)} \rceil + \lceil \log_2 r_B^{(\epsilon)} \rceil + \lceil \log_2 r_C^{(\epsilon)} \rceil.$$

Then

$$t_\epsilon(|\psi\rangle) \le \mathsf{QCorr}^{pure}_\epsilon(|\psi\rangle) \le t_{\epsilon/3}(|\psi\rangle).$$

It turns out that the relationship between $\mathsf{QCorr}_\epsilon(|\psi\rangle)$ and $\mathsf{QCorr}^{pure}_\epsilon(|\psi\rangle)$ can be characterized by the following theorem.

Theorem 1.10. *Let* $|\psi\rangle$ *be a pure state in* $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, *and* ϵ *is a small positive number. Then*

$$\frac{3}{4}\mathsf{QCorr}^{pure}_{3\epsilon}(|\psi\rangle) \le \mathsf{QCorr}_\epsilon(|\psi\rangle) \le \mathsf{QCorr}^{pure}_\epsilon(|\psi\rangle).$$

2 Preliminaries

Matrix theory. For a natural number n we let $[n]$ represent the set $\{1, 2, \ldots, n\}$. We sometimes write $A = [a_{x,y}]$ to mean that A is a matrix with the (x, y)-th entry being $a_{x,y}$. An operator A is said to be *Hermitian* if $A^\dagger = A$. A Hermitian operator A is said to be *positive semi-definite* (PSD) if all its eigenvalues are non-negative. For any vectors $|v_1\rangle, \ldots, |v_r\rangle$ in $\mathbb{C}^n$, the $r \times r$ matrix M defined by $M(i,j) \stackrel{\text{def}}{=} \langle v_i|v_j\rangle$ is positive semi-definite. The following definition of PSD-rank of a matrix was proposed in [8].

DEFINITION 2.1. *For a matrix $P \in \mathbb{R}_+^{n\times m}$, its PSD-rank, denoted $\mathtt{rank}^{(2)}_{\mathtt{psd}}(P)$, is the minimum number r such that there are PSD matrices $C_x, D_y \in \mathbb{C}^{r\times r}$ with $\mathtt{tr}(C_x D_y) = P(x, y)$, $\forall x \in [n], y \in [m]$.*

Quantum information. A quantum state ρ in Hilbert space $\mathcal{H}$, denoted $\rho \in \mathcal{H}$, is a trace one positive semi-definite operator acting on $\mathcal{H}$. A quantum state ρ is called *pure* if it is rank one, namely $\rho = |\psi\rangle\langle\psi|$ for some vector $|\psi\rangle$ of unit ℓ_2 norm; in this case, we often identify ρ with $|\psi\rangle$. For quantum states ρ and σ, their fidelity is defined as $\mathsf{F}(\rho, \sigma) \stackrel{\text{def}}{=} \mathtt{tr}(\sqrt{\sigma^{1/2}\rho\sigma^{1/2}})$. For $\rho, |\psi\rangle \in \mathcal{H}$, we have $\mathsf{F}(\rho, |\psi\rangle\langle\psi|) = \sqrt{\langle\psi|\rho|\psi\rangle}$. We define norm of $|\psi\rangle$ as $\||\psi\rangle\| \stackrel{\text{def}}{=} \sqrt{\langle\psi|\psi\rangle}$. For a quantum state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$, we let $\mathtt{tr}_{\mathcal{H}_B}\rho$ represent the partial trace of ρ in $\mathcal{H}_A$ after tracing out $\mathcal{H}_B$. Let $\rho \in \mathcal{H}_A$ and $|\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ be such that $\mathtt{tr}_{\mathcal{H}_B}|\phi\rangle\langle\phi| = \rho$, then we call $|\phi\rangle$ a *purification* of ρ.

DEFINITION 8. *For a pure state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$, its* Schmidt decomposition *is defined as*

$$|\psi\rangle = \sum_{i=1}^{r} \sqrt{p_i} \cdot |v_i\rangle \otimes |w_i\rangle,$$

where the states $|v_i\rangle \in \mathcal{H}_A$ are orthonormal, and so are the states $|w_i\rangle \in \mathcal{H}_B$, and p is a probability distribution.

It is easily seen that r is also equal to $\mathtt{rank}(\mathtt{tr}_{\mathcal{H}_A}|\psi\rangle\langle\psi|) = \mathtt{rank}(\mathtt{tr}_{\mathcal{H}_B}|\psi\rangle\langle\psi|)$ and is therefore the same in all Schmidt decompositions of $|\psi\rangle$. This number is also referred to as the *Schmidt rank* of $|\psi\rangle$ and denoted $\mathtt{S\text{-}rank}^{(A,B)}(|\psi\rangle)$. The next fact follows by considering Schmidt decomposition of the pure states involved; see, for example, Ex(2.81) of [6].

FACT 1. *Let $|\psi\rangle, |\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ be such that $\mathtt{tr}_{\mathcal{H}_B}|\phi\rangle\langle\phi| = \mathtt{tr}_{\mathcal{H}_B}|\psi\rangle\langle\psi|$. There exists a unitary operation U on $\mathcal{H}_B$ such that $(I_{\mathcal{H}_A} \otimes U)|\psi\rangle = |\phi\rangle$, where $I_{\mathcal{H}_A}$ is the identity operator on $\mathcal{H}_A$.*

We will also need another fundamental fact, shown by Uhlmann [6].

FACT 2. (UHLMANN, [6]) *Let $\rho, \sigma \in \mathcal{H}_A$. Let $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ be a purification of ρ and $\dim(\mathcal{H}_A) \leq \dim(\mathcal{H}_B)$. There exists a purification $|\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ of σ such that $\mathsf{F}(\rho, \sigma) = |\langle\phi|\psi\rangle|$.*

The approximate version of Schmidt decomposition that will be utilized in the present paper is as follows, which is called *approximate Schmidt rank.*

DEFINITION 2.2. *Let $\epsilon > 0$. Let $|\psi\rangle$ be a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B$. Define*

$$\begin{aligned} \mathtt{S\text{-}rank}_\epsilon^{(A,B)}(|\psi\rangle) \stackrel{\text{def}}{=} \min\{&\mathtt{S\text{-}rank}^{(A,B)}(|\phi\rangle) : |\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \\ &\textit{and } \mathsf{F}(|\psi\rangle\langle\psi|, |\phi\rangle\langle\phi|) \geq 1 - \epsilon\}. \end{aligned} \tag{2.8}$$

For multipartite pure states, usually there are no Schmidt decompositions. Instead, the following fact holds. Here we only prove it for the tripartite case, and it could be generalized to general cases easily.

LEMMA 2.1. *Suppose $|\psi\rangle$ is a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and ρ_A, ρ_B and ρ_C are the reduced density matrices of $|\psi\rangle$ in $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_C$ respectively. And assume $\{|\alpha_i\rangle\}$, $\{|\beta_j\rangle\}$, $\{|\gamma_k\rangle\}$ are the nonzero eigenvectors of ρ_A, ρ_B and ρ_C respectively. Then $|\psi\rangle$ can be expressed as*

$$|\psi\rangle = \sum_{ijk} a_{ijk} |\alpha_i\rangle |\beta_j\rangle |\gamma_k\rangle,$$

where a_{ijk}'s are complex coefficients.

Proof. Suppose the Schmidt decomposition of $|\psi\rangle$ with respect to the separation (A, BC) is

$$|\psi\rangle = \sum_i a_i |\alpha_i\rangle |\phi_i\rangle.$$

Besides, for any i let the Schmidt decomposition of $|\phi_i\rangle$ with respect to the separation (B, C) be

$$|\phi_i\rangle = \sum_j b_{ij} |\mu_{ij}\rangle |\nu_{ij}\rangle.$$

Thus, $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \sum_i \sum_j a_i b_{ij} |\alpha_i\rangle |\mu_{ij}\rangle |\nu_{ij}\rangle. \tag{2.9}$$

On the other hand, according to the definitions of ρ_B and ρ_C, we know that

$$\rho_B = \sum_i |a_i|^2 \mathtt{tr}_{\mathcal{H}_C} |\phi_i\rangle\langle\phi_i| = \sum_{ij} |a_i|^2 |b_{ij}|^2 |\mu_{ij}\rangle\langle\mu_{ij}| \tag{2.10}$$

and

$$\rho_C = \sum_i |a_i|^2 \mathtt{tr}_{\mathcal{H}_B} |\phi_i\rangle\langle\phi_i| = \sum_{ij} |a_i|^2 |b_{ij}|^2 |\nu_{ij}\rangle\langle\nu_{ij}|. \tag{2.11}$$

Eq (2.10) and Eq (2.11) indicate that for any i, j, $|\mu_{ij}\rangle$ is in the support of ρ_B, and $|\nu_{ij}\rangle$ is in the support of ρ_C. That is, for any i, j, $|\mu_{ij}\rangle$ and $|\nu_{ij}\rangle$ can always be linearly expressed by $\{|\beta_j\rangle\}$ and $\{|\gamma_k\rangle\}$ respectively. Recall that we have Eq (2.9), then the proof is completed.

3 Approximate Quantum Correlation Complexity of Bipartite States

In this section, we prove the theorems in Section 1.1. First we show that the two definitions of approximation are equivalent. Recall that for a state $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$,

$$\mathsf{QCorr}_\epsilon(\rho) = \min\{\mathsf{QCorr}(\rho') : \rho' \in \mathcal{H}_{AB}, \mathsf{F}(\rho, \rho') \geq 1 - \epsilon\},$$

and

$$\begin{aligned}\mathsf{QCorr}'_\epsilon(\rho) &= \min\left\{\mathsf{QCorr}^{pure}_\epsilon(|\phi\rangle) : |\varphi\rangle \in \mathcal{H}_{A_1ABB_1}, \rho = \mathtt{tr}_{\mathcal{H}_{A_1}\otimes\mathcal{H}_{B_1}} |\varphi\rangle\langle\varphi|\right\} \\ &= \min\left\{\lceil \log_2 \mathtt{S\text{-}rank}_\epsilon(|\varphi\rangle)\rceil : |\varphi\rangle \in \mathcal{H}_{A_1ABB_1}, \rho = \mathtt{tr}_{\mathcal{H}_{A_1}\otimes\mathcal{H}_{B_1}} |\varphi\rangle\langle\varphi|\right\}.\end{aligned}$$

LEMMA 3.1. (restatement of Lemma 1.1) *For any quantum state ρ in $\mathcal{H}_A \otimes \mathcal{H}_B$, $\mathsf{QCorr}_\epsilon(\rho) = \mathsf{QCorr}'_\epsilon(\rho)$.*

Proof $\mathsf{QCorr}_\epsilon(\rho) \geq \mathsf{QCorr}'_\epsilon(\rho)$: Suppose that $\rho' \in \mathcal{H}_A \otimes \mathcal{H}_B$, $\mathsf{F}(\rho, \rho') \geq 1-\epsilon$ and $\mathsf{QCorr}_\epsilon(\rho) = \mathsf{QCorr}(\rho')$. By Lemma 2.2 of [4], there is a purification $|\psi\rangle$ in A_1ABB_1 of ρ' *s.t.* $\mathsf{QCorr}(\rho') = \lceil \log_2 \texttt{S-rank}(|\psi\rangle) \rceil$. By Uhlmann's theorem, there exists a purification of ρ in A_1ABB_1, say $|\alpha\rangle$, and $\mathsf{F}(|\alpha\rangle\langle\alpha|, |\psi\rangle\langle\psi|) = \mathsf{F}(\rho, \rho') \geq 1 - \epsilon$. (We assume that the $|\alpha\rangle$ and $|\psi\rangle$ are in the same extended space $\mathcal{H}_{A_1ABB_1}$ since otherwise we can use the union of the two extended spaces.) Thus

$$\mathsf{QCorr}'_\epsilon(\rho) \leq \lceil \log_2 \texttt{S-rank}_\epsilon(|\alpha\rangle) \rceil \leq \lceil \log_2 \texttt{S-rank}(|\psi\rangle) \rceil \leq \mathsf{QCorr}_\epsilon(\rho).$$

$\mathsf{QCorr}_\epsilon(\rho) \leq \mathsf{QCorr}'_\epsilon(\rho)$: Suppose $\mathsf{QCorr}'_\epsilon(\rho) = \lceil \log_2 \texttt{S-rank}_\epsilon(|\varphi\rangle) \rceil$, and $\rho = \texttt{tr}_{\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1}} |\varphi\rangle\langle\varphi|$. By Lemma 3.3, one can find another pure state $|\beta\rangle$ in A_1ABB_1, such that $\lceil \log_2 \texttt{S-rank}(|\beta\rangle) \rceil = \lceil \log_2 \texttt{S-rank}_\epsilon(|\varphi\rangle) \rceil = \mathsf{QCorr}'_\epsilon(\rho)$, and $\mathsf{F}(|\beta\rangle\langle\beta|, |\varphi\rangle\langle\varphi|) \geq 1 - \epsilon$. Since partial trace does not decrease the fidelity [6], we know that $\mathsf{F}(\texttt{tr}_{\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1}} |\beta\rangle\langle\beta|, \rho) \geq 1 - \epsilon$. By the definition of $\mathsf{QCorr}_\epsilon(\rho)$, it holds that $\mathsf{QCorr}'_\epsilon(\rho) \geq \mathsf{QCorr}_\epsilon(\rho)$, which completes the proof. □

LEMMA 3.2. ([4]) *Consider an arbitrary nonnegative matrix P with $\sum_{x,y} P(x,y) = 1$.*

1. *Suppose that $|\psi\rangle$ is a purification of P in $\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1}$. We write its Schmidt decomposition as $|\psi\rangle = \sum_{i=1}^r \left(\sum_x |x\rangle \otimes |u_x^i\rangle \right) \otimes \left(\sum_y |y\rangle \otimes |v_y^i\rangle \right)$. Then the $r \times r$ complex-valued matrices $\{C_x\}$ and $\{D_y\}$ defined by $C_x(i,j) = \langle u_{x,i} | u_{x,j} \rangle$ and $D_y(i,j) = \langle v_{y,i} | v_{y,j} \rangle$ are positive semi-definite, and $P(x,y) = \langle C_x, D_y \rangle$.*
2. *For any $r \times r$ PSD-decomposition $\{C_x, D_y : x, y\}$ of P, suppose that the j-th column of $\sqrt{C_x}$ is $|u_{x,j}\rangle$ and the j-th column of $\sqrt{D_y}$ is $|v_{y,j}\rangle$, then the state defined by $|\psi\rangle = \sum_{i=1}^r \left(\sum_x |x\rangle \otimes |u_x^i\rangle \right) \otimes \left(\sum_y |y\rangle \otimes |v_y^i\rangle \right)$ is a purification of P and $\texttt{S-rank}(|\psi\rangle) \leq r$.*

DEFINITION 9. *For an nonnegative matrix $P \in \mathbb{R}_+^{M \times N}$ with $\sum_{x,y} P(x,y) = 1$, its ϵ-error psd-rank, denoted $\texttt{rank}_{\texttt{psd},\epsilon}(P)$, is the minimum number r s.t. P has a PSD-decomposition $C_x, D_y \in \mathbb{C}^{s \times s}$ ($s \geq r$) with the r largest $(\sum_x C_x)_{i,i} (\sum_y D_y)_{i,i}$ (over all $i \in [s]$) sum up to at least $1 - \epsilon$.*

Note that this definition is different from the approximate PSD-rank in Definition 2, but very soon we will see that they are actually equivalent.

LEMMA 3.3. ([4]) *For a bipartite pure state $|\psi\rangle$ with Schmidt coefficients $\lambda_1 \geq ... \geq \lambda_N$, $\mathsf{QCorr}_\epsilon(|\psi\rangle) = \mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle) = \lceil \log_2 r \rceil$, where r is the minimum integer s.t. $\sum_{i=1}^r \lambda_i^2 \geq (1-\epsilon)^2$.*

This lemma implies that the most efficient approximate generation of a pure state can be achieved by another pure state. In the same spirit, the following theorem shows that the most efficient approximate generation of a classical state can be achieved by another classical state, and the correlation complexity is completely determined by the approximate PSD-rank.

THEOREM 3.1. (Theorem 1.1) *For any classical state P,*

$$\mathsf{QCorr}_\epsilon(P) = \mathsf{QCorr}_\epsilon^{cla}(P) = \lceil \log_2 \texttt{rank}_{\texttt{psd}}^{(2),\epsilon}(P) \rceil.$$

Proof We will first prove $\mathsf{QCorr}_\epsilon(P) = \lceil \log_2 \texttt{rank}_{\texttt{psd},\epsilon}(P) \rceil$. For any purification $|\psi\rangle$ of of P, there are corresponding matrices $\{C_x\}$ and $\{D_y\}$ from Lemma 3.2. Put $C = \sum_x C_x$ and $D = \sum_y D_y$. The Schmidt coefficients of $|\psi\rangle$ are

$$\lambda_i(|\psi\rangle) = \left(\sum_x \| |u_{x,i}\rangle \|^2 \right) \left(\sum_y \| |v_{y,i}\rangle \|^2 \right) = \left(\sum_x C_x(i,i) \right) \left(\sum_y D_y(i,i) \right) = C(i,i) D(i,i)$$

Without loss of generality, we can assume that these λ_i's are in decreasing order.

$$\begin{aligned}
\mathsf{QCorr}_\epsilon(P) &= \mathsf{QCorr}'_\epsilon(P) && \text{(Lemma 3.1)}\\
&= \min\{\mathsf{QCorr}_\epsilon(|\psi\rangle) : |\psi\rangle \text{ purifies } P\} && \text{(Def of } \mathsf{QCorr}'_\epsilon)\\
&= \min\left\{\lceil \log_2 r\rceil : \sum_{i=1}^{r} \lambda_i(|\psi\rangle)^2 \geq (1-\epsilon)^2, |\psi\rangle \text{ purifies } P\right\} && \text{(Lemma 3.3)}\\
&= \lceil \log_2 \mathtt{rank}_{\mathtt{psd},\epsilon}(P)\rceil && \text{(Def of } \epsilon\text{-error psd-rank)}
\end{aligned}$$

Next we prove $\mathsf{QCorr}_\epsilon(P) = \mathsf{QCorr}^{cla}_\epsilon(P)$.

$$\begin{aligned}
\mathsf{QCorr}_\epsilon(P) &= \min\{\mathsf{QCorr}_\epsilon(|\psi\rangle) : |\psi\rangle \text{ purifies } P\} && \text{(Def of } \mathsf{QCorr}'_\epsilon)\\
&= \min\{\mathsf{QCorr}^{pure}_\epsilon(|\psi\rangle) : |\psi\rangle \text{ purifies } P\} && \text{(Lemma 3.3)}\\
&= \min\{\mathsf{QCorr}(|\psi'\rangle) : \mathsf{F}(|\psi\rangle, |\psi'\rangle) \geq 1-\epsilon, |\psi\rangle \text{ purifies } P\} && \text{(Def of } \mathsf{QCorr}^{pure}_\epsilon)\\
&= \min\{\mathsf{QCorr}(|\bar{\psi}'\rangle) : \mathsf{F}(|\bar{\psi}\rangle, |\bar{\psi}'\rangle) \geq 1-\epsilon, |\bar{\psi}\rangle \text{ purifies } P\}\\
&\geq \min\{\mathsf{QCorr}(P') : \mathsf{F}(|\bar{\psi}\rangle, |\bar{\psi}'\rangle) \geq 1-\epsilon, |\bar{\psi}\rangle \text{ purifies } P, |\bar{\psi}'\rangle \text{ purifies } P'\}\\
&\geq \min\{\mathsf{QCorr}(P') : \mathsf{F}(P, P') \geq 1-\epsilon\}\\
&= \mathsf{QCorr}^{cla}_\epsilon(P),
\end{aligned}$$

where $|\bar{\psi}\rangle$ is in $\mathcal{H}_A \otimes \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1}$, and can be expressed as

$$|\bar{\psi}\rangle \stackrel{\text{def}}{=} \sum_i \Big(\sum_x |x\rangle \otimes |x\rangle \otimes |v^i_x\rangle\Big) \otimes \Big(\sum_y |y\rangle \otimes |y\rangle \otimes |w^i_y\rangle\Big).$$

Similarly, $|\bar{\psi}'\rangle$ has the same relation with $|\psi'\rangle$. Then it can be checked that $|\bar{\psi}\rangle$ does purify P, and $\mathtt{tr}_{\mathcal{H}_A\otimes\mathcal{H}_{A_1}\otimes\mathcal{H}_B\otimes\mathcal{H}_{B_1}} |\psi'\rangle\langle\psi'|$ is another classical state. We let the corresponding distribution be P'.

To see the first inequality above, note that $|\psi'\rangle$ is one purification of P', thus $\mathsf{QCorr}(P') \leq \mathsf{QCorr}(|\bar{\psi}'\rangle)$. To see the last inequality, note that $\mathsf{F}(P, P') \geq \mathsf{F}(|\bar{\psi}\rangle, |\bar{\psi}'\rangle)$ since partial trace does not decrease fidelity. Meanwhile, according to the definition of $\mathsf{QCorr}^{cla}_\epsilon(P)$ it is easy to see that $\mathsf{QCorr}_\epsilon(P) \leq \mathsf{QCorr}^{cla}_\epsilon(P)$, which means that $\mathsf{QCorr}_\epsilon(P) = \mathsf{QCorr}^{cla}_\epsilon(P)$.

On the other hand, according to the fact that $\mathsf{QCorr}(P) = \lceil \log_2 \mathtt{rank}^{(2)}_{\mathtt{psd}}(P)\rceil$ proved in [4] and the definition of $\mathtt{rank}^{(2),\epsilon}_{\mathtt{psd}}(P)$, it holds that $\mathsf{QCorr}^{cla}_\epsilon(P) = \min\{\lceil \log_2 \mathtt{rank}^{(2)}_{\mathtt{psd}}(P')\rceil : F(P, P') \geq 1-\epsilon, P' \text{ is another classical state in } \mathcal{H}_A \otimes \mathcal{H}_B\} = \lceil \log_2 \mathtt{rank}^{(2),\epsilon}_{\mathtt{psd}}(P)\rceil$.

Put all the three results above together, we complete the proof. □

We now turn to the case of general bipartite σ. By combining Theorem 1.2 of [4] and Lemma 3.1, we have the following characterization of $\mathsf{QCorr}_\epsilon(\sigma)$.

Theorem 3.2. (Theorem 1.2) *Let σ be an arbitrary quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B$, and $0 < \epsilon < 1$. Let $|x\rangle$, $|x'\rangle$ range over the computational basis states for $\mathcal{H}_A$, and $|y\rangle$, $|y'\rangle$ for $\mathcal{H}_B$. $\{A_x\}$'s and $\{B_y\}$'s are matrices with the same column number l that makes*

$$\sigma = \sum_{x,x';y,y'} |x\rangle\langle x'| \otimes |y\rangle\langle y'| \cdot \mathtt{tr}\Big((A^\dagger_{x'} A_x)^T (B^\dagger_{y'} B_y)\Big). \tag{3.12}$$

For any $0 < \epsilon < 1$, suppose r is the minimum number taken over all possible $\{A_x\}$'s and $\{B_y\}$'s such that for $i \neq j$,

$$\sum_x \langle A_x(i)|A_x(j)\rangle = \sum_y \langle B_y(i)|B_y(j)\rangle = 0, \tag{3.13}$$

and

$$\sum_{i=1}^{r}\Big(\sum_{x}\langle A_x(i)|A_x(i)\rangle\Big)\Big(\sum_{y}\langle B_y(i)|B_y(i)\rangle\Big) \geq 1-\epsilon, \tag{3.14}$$

where for convenience, we denote the i-th column of any matrix A by $|A(i)\rangle$. *Then* $\mathsf{QCorr}_\epsilon(\sigma) = \lceil \log_2 r \rceil$.

Proof. Suppose $\mathsf{QCorr}_\epsilon(\sigma) = \lceil \log_2 t \rceil$, then according to Lemma 3.1 there exists a purification of σ in $\mathcal{H}_{A_1}\otimes\mathcal{H}_A\otimes\mathcal{H}_B\otimes\mathcal{H}_{B_1}$, denoted $|\psi\rangle$, such that $\texttt{S-rank}_\epsilon(|\psi\rangle) = t$. Suppose the Schmidt decomposition of $|\psi\rangle$ is

$$|\psi\rangle = \sum_{i=1}^{s}\Big(\sum_{x}|x\rangle\otimes|v_x^i\rangle\Big)\otimes\Big(\sum_{y}|y\rangle\otimes|w_y^i\rangle\Big), \tag{3.15}$$

thus the Schmidt coefficients are $a_i = \sum_x \langle v_x^i|v_x^i\rangle \sum_y \langle w_y^i|w_y^i\rangle$, $1 \leq i \leq s$. For each x, set matrices $A_x \overset{\text{def}}{=} (|v_x^1\rangle, |v_x^2\rangle, \ldots, |v_x^s\rangle)$. Similarly, for each y set matrices $B_y \overset{\text{def}}{=} (|w_y^1\rangle, |w_y^2\rangle, \ldots, |w_y^s\rangle)$. Then it can be verified that Eq.(3.12) holds. Without loss of generality, we assure $a_{j_1} \geq a_{j_2}$ for any $j_1 > j_2$, otherwise we could achieve this by adjusting the index i of Eq.(3.15). Then by Lemma 5.1 of [4], we have that

$$\sum_{i=1}^{t} a_i = \sum_{i=1}^{t}\Big(\sum_{x}\langle A_x(i)|A_x(i)\rangle\Big)\Big(\sum_{y}\langle B_y(i)|B_y(i)\rangle\Big) \geq 1-\epsilon.$$

At the same time, according to the definition of Schmidt decomposition, it holds that for $i \neq j$, $\sum_x \langle A_x(i)|A_x(j)\rangle = \sum_y \langle B_y(i)|B_y(j)\rangle = 0$, which indicates that $r \leq t$, and $\mathsf{QCorr}_\epsilon(\sigma) \geq \lceil \log_2 r \rceil$.

On the other hand, assume that $\{A_x\}$'s and $\{B_y\}$'s are matrices that satisfy the requirements from Eq.(3.12) to Eq.(3.14). Then it can be verified that

$$|\tilde{\psi}\rangle = \sum_{i=1}^{l}\Big(\sum_{x}|x\rangle\otimes|A_x(i)\rangle\Big)\otimes\Big(\sum_{y}|y\rangle\otimes|B_y(i)\rangle\Big) \tag{3.16}$$

is a purification of σ in $\mathcal{H}_{A_1}\otimes\mathcal{H}_A\otimes\mathcal{H}_B\otimes\mathcal{H}_{B_1}$. Besides, suppose

$$|\tilde{\psi}'\rangle = \sum_{i=1}^{r}\Big(\sum_{x}|x\rangle\otimes|A_x(i)\rangle\Big)\otimes\Big(\sum_{y}|y\rangle\otimes|B_y(i)\rangle\Big), \tag{3.17}$$

then Eq.(3.13) and Eq.(3.14) means that $|\langle\tilde{\psi}|\tilde{\psi}'\rangle| \geq 1-\epsilon$. Since $\texttt{S-rank}(|\tilde{\psi}'\rangle) \leq r$, it holds that $\texttt{S-rank}_\epsilon(|\tilde{\psi}\rangle) \leq r$, and according to Lemma 3.1 we know that $\mathsf{QCorr}_\epsilon(\sigma) \leq \lceil \log_2 r \rceil$, which completes the proof.

4 Quantum Correlation Complexity of Multipartite States

In this section, we prove the results in Subsection 1.2.

THEOREM 4.1. (Theorem 1.3) *Suppose* $|\psi\rangle$ *is a pure state in* $\mathcal{H}_A\otimes\mathcal{H}_B\otimes\mathcal{H}_C$, *and* ρ_A, ρ_B *and* ρ_C *are the reduced density matrices of* $|\psi\rangle$ *in* $\mathcal{H}_A$, $\mathcal{H}_B$ *and* $\mathcal{H}_C$ *respectively. Assume*

$$t(|\psi\rangle) = \lceil \log_2 r_A \rceil + \lceil \log_2 r_B \rceil + \lceil \log_2 r_C \rceil,$$

where r_i *is the rank of* $\rho_i (i = A, B, C)$. *Then we have that*

$$\mathsf{QCorr}(|\psi\rangle) = t(|\psi\rangle).$$

Proof. According to Lemma 2.1, suppose $|\psi\rangle = \sum_{ijk} a_{ijk}|\alpha_i\rangle|\beta_j\rangle|\gamma_k\rangle$, then Alice, Bob, and Charlie can generate $|\psi\rangle$ by local operations on the seed state $|\psi'\rangle = \sum_{ijk} a_{ijk}|i\rangle|j\rangle|k\rangle$, which means that $\mathsf{QCorr}(|\psi\rangle) \leq t$.

For the other direction, let us assume the three players could generate the target $|\psi\rangle$ by local operations on an initial seed state σ, and according to the definition of quantum correlation complexity, we could suppose the size of σ is $\mathsf{QCorr}(|\psi\rangle)$. Note that it is possible that σ is a mixed state. However, considering the linearity of quantum operations and the fact that the target state is pure, we could choose σ as a pure state. Now define the reduced density matrices of σ in the three systems as σ_A, σ_B and σ_C respectively. Suppose the ranks of them are s_A, s_B and s_C. Then we have $\mathsf{QCorr}(|\psi\rangle) \geq \lceil \log_2 s_A \rceil + \lceil \log_2 s_B \rceil + \lceil \log_2 s_C \rceil$, as the number of qubits in σ_i is at least $\lceil \log_2 s_i \rceil$, where $i = A, B, C$. On the other hand, it can be seen that s_A is essentially the Schmidt rank of σ with respect to the separation (A, BC). Besides, the local operations performed by Alice to generate $|\psi\rangle$ cannot change the Schmidt rank with respect to this separation, and similar conclusion also holds for the separations (AB, C) and (AC, B). As a result, $s_A = r_A$, $s_B = r_B$, and $s_C = r_C$, which means that $\mathsf{QCorr}(|\psi\rangle) \geq \lceil \log_2 r_A \rceil + \lceil \log_2 r_B \rceil + \lceil \log_2 r_C \rceil = t(|\psi\rangle)$. Combining the two directions, we have that $\mathsf{QCorr}(|\psi\rangle) = t(|\psi\rangle)$.

The above theorem could be generalized straightforward to arbitrary multipartite pure states.

THEOREM 4.2. *Suppose $|\psi\rangle$ is a k-partite pure state in $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_k$. Suppose for any $i \in [k]$, ρ_i is the reduced density matrices of $|\psi\rangle$ in $\mathcal{H}_i$, and r_i is the rank of ρ_i. Assume*

$$t(|\psi\rangle) = \sum_{i=1}^{k} \lceil \log_2 r_i \rceil.$$

Then we have that

$$\mathsf{QCorr}(|\psi\rangle) = t(|\psi\rangle).$$

Note that when $k = 2$, Theorem 4.2 goes back exactly to the bipartite case discussed in [4], where $r_1 = r_2 = r$, and it is actually the Schmidt rank of $|\psi\rangle$.

The following theorem characterizes the relationship between quantum correlation complexity of a general multipartite ρ and that of its purifications.

THEOREM 4.3. (Theorem 1.4) *Assume that ρ is a quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and $r(\rho)$ is defined as in Eq.*(1.6). *Then we have*

$$\mathsf{QCorr}(\rho) \leq r(\rho) \leq \frac{4}{3}\mathsf{QCorr}(\rho).$$

Proof. First, we have $\mathsf{QCorr}(\rho) \leq \mathsf{QCorr}(|\psi\rangle)$ for any purification $|\psi\rangle$ of ρ in $\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$, thus $\mathsf{QCorr}(\rho) \leq r(\rho)$.

For the other direction, suppose the minimal seed state for generating ρ is σ, and generally σ is a mixed state with size $\mathsf{QCorr}(\rho)$. Let σ_A, σ_B and σ_C are the reduced density matrices of σ in the space of Alice, Bob, and Charlie respectively. Suppose n_A, n_B and n_C are the numbers of qubits of σ_A, σ_B and σ_C respectively, then $\mathsf{QCorr}(\rho) = n_A + n_B + n_C$. Without loss of generality, we suppose $n_A \leq n_B \leq n_C$. Note that we can always find a purification $|\theta\rangle$ of σ in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_2}$. Starting from $|\theta\rangle$, we could generate a purification $|\psi\rangle$ of ρ in $\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ by local operations. In this way, $\mathsf{QCorr}(|\psi\rangle) \leq \mathsf{QCorr}(|\theta\rangle)$. According to Theorem 4.1, if the dimensions of σ_A, σ_B and σ'_C are r_A,

r_B and r_C, then $\mathsf{QCorr}(|\theta\rangle) = \lceil \log_2 r_A \rceil + \lceil \log_2 r_B \rceil + \lceil \log_2 r_C \rceil$, where $\sigma'_C = \mathtt{tr}_{\mathcal{H}_A \otimes \mathcal{H}_B} |\theta\rangle\langle\theta|$. Moreover, we have $r_A \leq 2^{n_A}$, $r_B \leq 2^{n_B}$, and $r_C \leq 2^{n_A+n_B}$, where the last inequality uses the fact that $|\theta\rangle$ is a pure state. Thus, it holds that

$$\mathsf{QCorr}(|\psi\rangle) \leq \mathsf{QCorr}(|\theta\rangle) \leq n_A + n_B + n_A + n_B \leq \frac{4}{3}(n_A + n_B + n_C) = \frac{4}{3}\mathsf{QCorr}(\rho).$$

That is, we eventually have that $r(\rho) \leq \frac{4}{3}\mathsf{QCorr}(\rho)$, and this completes the proof.

The following lemma shows that $r(\rho)$ could be strictly larger than $\mathsf{QCorr}(\rho)$.

LEMMA 4.1. $\rho_0 = \frac{1}{2}|GHZ\rangle\langle GHZ| + \frac{1}{2}|W\rangle\langle W|$, *then* $r(\rho_0) = 4$.

Proof. Suppose the three qubits of ρ_0 are possessed by Alice, Bob, and Charlie respectively. For convenience, we call these three qubits the main system. Then an arbitrary purification of ρ_0 in $\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ could be expressed as

$$|\psi\rangle = \frac{1}{\sqrt{2}}|GHZ\rangle|u_0\rangle + \frac{1}{\sqrt{2}}|W\rangle|u_1\rangle,$$

where $|u_0\rangle$ and $|u_1\rangle$ are orthogonal, and they are composed by all the ancillary systems introduced by the three players. Note that it is possible that some of the players do not have ancillary systems. Without loss of generality, we suppose some of the qubits in $|u_i\rangle$ belong to Alice. We trace out the two qubits of Bob and Charlie in the main systems from $|\psi\rangle$, and get

$$\begin{aligned}\rho_a =& \mathtt{tr}_{\mathcal{H}_B \otimes \mathcal{H}_C} |\psi\rangle\langle\psi| \\ =& \left(\frac{1}{2}|0\rangle|u_0\rangle + \frac{1}{\sqrt{6}}|1\rangle|u_1\rangle\right)\left(\frac{1}{2}\langle 0|\langle u_0| + \frac{1}{\sqrt{6}}\langle 1|\langle u_1|\right) \\ &+ \frac{1}{4}|1\rangle\langle 1| \otimes |u_0\rangle\langle u_0| + \frac{1}{3}|0\rangle\langle 0| \otimes |u_1\rangle\langle u_1|,\end{aligned}$$

where the first qubit belongs to Alice, and the rest is all the ancillary systems combined. Continue to trace out Bob's ancillary system and Charlie's ancillary system, then we obtain Alice's reduced density matrix ρ'_a. Similarly, we can define ρ'_b or ρ'_c, provided Bob or Charlie has a nontrivial part in $|u_i\rangle$.

We now prove that at least one of ρ'_a, ρ'_b and ρ'_c have a rank at least 3. If this is the case, it is not difficult to know that $\mathsf{QCorr}(|\psi\rangle) \geq 4$. At the same time, consider a special purification $|\psi_0\rangle$ of ρ_0

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|GHZ\rangle|0\rangle + \frac{1}{\sqrt{2}}|W\rangle|1\rangle,$$

where the last qubit is introduced by Charlie as an ancillary system. By straightforward calculation, it can be verified that $\mathsf{QCorr}(|\psi_0\rangle) = 4$, which means that $r(\rho_0) = 4$.

To prove this conclusion, we first look at the possibility that only Alice introduces an ancillary system. In this case, actually it holds that $\rho'_a = \rho_a$, and it is clear that ρ'_a has a rank 3. If more than Alice introduces ancillary systems, we claim that if $|u_0\rangle$ or $|u_1\rangle$ is not a product state, one of ρ'_a, ρ'_b and ρ'_c must have a rank at least 3. For instance, suppose $|u_0\rangle$ is not a product state, then there must be some player, say Alice, such that the reduced density matrix of $|\psi\rangle$ on its ancillary system has a rank larger than 1, i.e., $\mathtt{rank}(\mathtt{tr}_{\mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |u_0\rangle\langle u_0|) \geq 2$. Note that $\mathtt{rank}(\rho'_a) \geq \mathtt{rank}(\mathtt{tr}_{\mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |u_0\rangle\langle u_0|) + \mathtt{rank}(\mathtt{tr}_{\mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |u_1\rangle\langle u_1|)$, where we have utilized the expression of ρ_a, and this means $\mathtt{rank}(\rho'_a) \geq 3$. Therefore, we only need to take care of the situation where $|u_0\rangle$ and $|u_1\rangle$ are product states. Since they are orthogonal, without loss of generality we could express them as $|u_0\rangle = |u_{0,a}\rangle|v_{0,bc}\rangle$ and $|u_1\rangle = |u_{1,a}\rangle|v_{1,bc}\rangle$, where $|u_{0,a}\rangle$ and $|u_{1,a}\rangle$ are two orthogonal states in $\mathcal{H}_{A_1}$, and $|v_{0,bc}\rangle$ and $|v_{1,bc}\rangle$ are in $\mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}$ or only one of them. In this way,

$$|\psi\rangle = \frac{1}{2}(|000\rangle + |111\rangle)|u_{0,a}\rangle|v_{0,bc}\rangle + \frac{1}{\sqrt{6}}(|001\rangle + |010\rangle + |001\rangle)|u_{1,a}\rangle|v_{1,bc}\rangle.$$

It is not difficult to verify that the rank of $\rho'_{bc} = \mathtt{tr}_{\mathcal{H}_A \otimes \mathcal{H}_{A_1}} |\psi\rangle\langle\psi|$ is at least 3. Meanwhile, it holds that $\mathtt{rank}(\rho'_{bc}) = \mathtt{rank}(\rho'_a)$. Hence, $\mathtt{rank}(\rho'_a) \geq 3$, and this completes the proof.

Generalizing Theorem 4.3 to general multipartite cases, we get the following result.

Theorem 4.4. *Assume that ρ is a k-partite quantum state in $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_k$, and $|\psi\rangle$ is a purification of ρ. Suppose $r(\rho) = \min_{|\psi\rangle} \mathsf{QCorr}(|\psi\rangle)$, then we have*

$$\mathsf{QCorr}(\rho) \leq r(\rho) \leq \frac{2k-2}{k} \mathsf{QCorr}(\rho).$$

When ρ is a multipartite classical state, it corresponds to a multipartite probability distribution. The following theorem characterize $\mathsf{QCorr}(\rho)$ for this case. And for simplicity, we only discuss the tripartite case.

Theorem 4.5. (Theorem 1.5) *Suppose $P = [P(x, y, z)]_{x,y,z}$ is a probability distribution on $\mathcal{X} \times \mathcal{Y} \times \mathcal{Z}$. Let*

$$\rho = \sum_{x,y,z} P(x, y, z)|x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z|.$$

Then we have

$$\frac{3}{4} \left\lceil \log_2 \mathtt{rank}^{(3)}_{\mathtt{psd}}(P) \right\rceil \leq \mathsf{QCorr}(\rho) \leq 3 \left\lceil \log_2 \mathtt{rank}^{(3)}_{\mathtt{psd}}(P) \right\rceil.$$

Proof. Let $r = \mathtt{rank}^{(3)}_{\mathtt{psd}}(P)$. Then we can find positive semi-definite matrices $\{C_x\}$, $\{D_y\}$ and $\{E_z\}$ such that for any x, y, z it holds that $P(x, y, z) = \sum_{i,j=1}^r C_x(i, j)D_y(i, j)E_z(i, j)$. For $i \in [r]$, let $|u^i_x\rangle$ be the i-th column of $\sqrt{C_x}$, $|v^i_y\rangle$ be the i-th column of $\sqrt{D_y}$, and $|w^i_z\rangle$ be the i-th column of $\sqrt{E_z}$. Then we have that $\langle u^j_x|u^i_x\rangle = C_x(i, j)$, $\langle v^j_y|v^i_y\rangle = D_y(i, j)$, and $\langle w^j_z|w^i_z\rangle = E_z(i, j)$. We now define a pure state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ as follows.

$$|\psi\rangle = \sum_{i=1}^r \left(\sum_x |x\rangle \otimes |x\rangle \otimes |u^i_x\rangle \right) \otimes \left(\sum_y |y\rangle \otimes |y\rangle \otimes |v^i_y\rangle \right) \otimes \left(\sum_z |z\rangle \otimes |z\rangle \otimes |w^i_z\rangle \right).$$

It can be checked that

$$\begin{aligned}
&\mathtt{tr}_{\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}} |\psi\rangle\langle\psi| \\
&= \sum_{x,y,z} |x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z| \left(\sum_{i,j=1}^r \langle u^j_x|u^i_x\rangle\langle v^j_y|v^i_y\rangle\langle w^j_z|w^i_z\rangle \right) \\
&= \sum_{x,y,z} P(x, y, z)|x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z| \quad = \quad \rho.
\end{aligned}$$

Thus $|\psi\rangle$ is actually a purification of ρ, and Theorem 4.3 points out that $\mathsf{QCorr}(\rho) \leq \mathsf{QCorr}(|\psi\rangle)$. Meanwhile, according to Theorem 4.1, it holds that $\mathsf{QCorr}(|\psi\rangle) \leq 3\lceil \log_2 r \rceil$. As a result, we obtain that $\mathsf{QCorr}(\rho) \leq 3\lceil \log_2 \mathtt{rank}_{\mathtt{psd}}^{(3)}(P) \rceil$.

On the other hand, suppose $|\psi'\rangle$ is the pure state in $\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ that achieves the optimum in Eq (1.6), then Theorem 4.3 tells us that

$$\mathsf{QCorr}(\rho) \geq \frac{3}{4}\mathsf{QCorr}(|\psi'\rangle) = \frac{3}{4}(\lceil \log_2 r_A \rceil + \lceil \log_2 r_B \rceil + \lceil \log_2 r_C \rceil) \geq \frac{3\log_2(r_A r_B r_C)}{4}, \tag{4.18}$$

where $r_i (i = A, B, C)$ are the dimensions of the reduced density matrices of $|\psi'\rangle$ on Alice, Bob, and Charlie respectively. According to Lemma 2.1, $|\psi'\rangle$ could be expressed as

$$|\psi'\rangle = \sum_{i=1}^{t} a_i |\alpha_i\rangle|\beta_i\rangle|\gamma_i\rangle.$$

Here $t = r_A r_B r_C$, and for $i \in [t]$, $|\alpha_i\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{A_1}$, $|\beta_i\rangle \in \mathcal{H}_B \otimes \mathcal{H}_{B_1}$, $|\gamma_i\rangle \in \mathcal{H}_C \otimes \mathcal{H}_{C_1}$. It should be pointed out that for different i and j, $|\alpha_i\rangle$ and $|\alpha_j\rangle$ might be the same, and the similar situation holds for $|\beta_i\rangle$ and $|\gamma_i\rangle$. In this way, $|\psi'\rangle$ could also be written as

$$|\psi'\rangle = \sum_{i=1}^{t} \left(\sum_x |x\rangle \otimes |u_x^i\rangle \right) \otimes \left(\sum_y |y\rangle \otimes |v_y^i\rangle \right) \otimes \left(\sum_z |z\rangle \otimes |w_z^i\rangle \right).$$

Recall that $|\psi'\rangle$ is a purification of ρ, so

$$\begin{aligned} \rho =& \mathtt{tr}_{\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |\psi'\rangle\langle\psi'| \\ =& \sum_{x,y,z} |x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z| \left(\sum_{i,j=1}^{t} \langle u_x^j | u_x^i \rangle \langle v_y^j | v_y^i \rangle \langle w_z^j | w_z^i \rangle \right) \\ =& \sum_{x,y,z} P(x,y,z) |x\rangle\langle x| \otimes |y\rangle\langle y| \otimes |z\rangle\langle z|. \end{aligned}$$

Note that for any x, the $t \times t$ matrix C_x with $C_x(j,i) = \langle u_x^j | u_x^i \rangle$ is positive, and similarly for any y and any z, we could define positive semi-definite matrices D_y with $D_y(j,i) = \langle v_y^j | v_y^i \rangle$, and E_z with $E_z(j,i) = \langle w_z^j | w_z^i \rangle$. Then the definition of psd-rank shows that $\mathtt{rank}_{\mathtt{psd}}^{(3)}(P) \leq t = r_A r_B r_C$. Combining this result with Eq.(4.18), we get that $\mathsf{QCorr}(\rho) \geq \frac{3}{4}\lceil \log_2 \mathtt{rank}_{\mathtt{psd}}^{(3)}(P) \rceil$, which completes the proof.

5 Quantum Communication Complexity of Multipartite States

In this section, we prove the results in Subsection 1.3.

Theorem 5.1. (Theorem 1.6) *Suppose $|\psi\rangle$ is a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and ρ_A, ρ_B and ρ_C are the reduced density matrices of $|\psi\rangle$ in $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}_C$ respectively. Assume*

$$t(|\psi\rangle) = \lceil \log_2 r_A \rceil + \lceil \log_2 r_B \rceil + \lceil \log_2 r_C \rceil,$$

where r_i is the rank of $\rho_i (i = A, B, C)$. Then we have that

$$\frac{1}{2} t(|\psi\rangle) \leq \mathsf{QComm}(|\psi\rangle) \leq \frac{2}{3} t(|\psi\rangle),$$

and both of the two inequalities could be tight.

Proof. First, it is not difficult to see that for any ρ in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, we have $\mathsf{QComm}(\rho) \leq \frac{2}{3}Q(\rho)$. Suppose Alice, Bob, and Charlie could generate ρ by local operations on the seed state σ, then one of them can prepare the seed state locally and then share it with the other two players by quantum communications. According to Theorem 4.1, we get that $\mathsf{QComm}(|\psi\rangle) \leq \frac{2}{3}t(|\psi\rangle)$.

For the other direction, suppose the amount of communication happened between Alice and Bob in the optimal communication scheme generating $|\psi\rangle$ is c_{AB} qubits, and similarly we define c_{AC} and c_{BC}. We now consider the quantum communication complexity of $|\psi\rangle$, $\mathsf{QComm}(|\psi\rangle)$, which means that the three players could start with some product state, and generate $|\psi\rangle$ by only local operations and quantum communication of $\mathsf{QComm}(|\psi\rangle)$ qubits. Again, considering the linearity of quantum operations, we could suppose the initial state is a product pure state. We now divide all the pure states involved into two parts: one is possessed by Alice, and the other is possessed by Bob and Charlie. Since exchanging r qubits can only increase the Schmidt rank by at most 2^r, we have that

$$r_A \leq 2^{c_{AB}+c_{AC}},$$

where we have used the conclusion that the Schmidt rank of $|\psi\rangle$ with respect of the separation (A, BC) is r_A, and similarly, it holds that

$$r_B \leq 2^{c_{AB}+c_{BC}}$$

and

$$r_C \leq 2^{c_{BC}+c_{AC}}.$$

Then we obtain that

$$\mathsf{QComm}(|\psi\rangle) = c_{AB} + c_{AC} + c_{BC} \geq \frac{1}{2}\left(\lceil \log_2 r_A \rceil + \lceil \log_2 r_B \rceil + \lceil \log_2 r_C \rceil\right) = \frac{1}{2}t(|\psi\rangle).$$

As an example, suppose $|\psi\rangle$ is the 3-qubit GHZ state shared by Alice, Bob and Charlie, then $t = 3$ and $\mathsf{QComm}(|\psi\rangle) = 2$, so the upper bound could be tight. On the other hand, consider the special case of $|\psi\rangle$ shared by only two of the three players, we could easily find an example where the lower bound is tight. The proof is completed.

Generalizing the above result to arbitrary multipartite cases, we have the following theorem.

THEOREM 5.2. *Suppose $|\psi\rangle$ is a k-partite pure state, and $t(|\psi\rangle)$ is defined as in Theorem 4.2. Then we have that*

$$\frac{1}{2}t(|\psi\rangle) \leq \mathsf{QComm}(|\psi\rangle) \leq \frac{k-1}{k}t(|\psi\rangle).$$

The following theorem shows a nice property of quantum communication complexity.

THEOREM 5.3. (Theorem 1.7) *Assume that ρ is a quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. Then*

$$\mathsf{QComm}(\rho) = \min_{\mathcal{H}_{A_1},\mathcal{H}_{B_1},\mathcal{H}_{C_1}} \{\mathsf{QComm}(|\psi\rangle) : |\psi\rangle \textit{ is a pure state}$$
$$\textit{in } \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}, \rho = \mathtt{tr}_{\mathcal{H}_{A_1}\otimes\mathcal{H}_{B_1}\otimes\mathcal{H}_{C_1}} |\psi\rangle\langle\psi|\}.$$

Proof. Let ρ be a quantum state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. First, suppose $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ is an arbitrary purification of ρ. It can be seen that $\mathsf{QComm}(\rho) \leq \mathsf{QComm}(|\psi\rangle)$, thus we have

$$\mathsf{QComm}(\rho) \leq \min_{\mathcal{H}_{A_1},\mathcal{H}_{B_1},\mathcal{H}_{C_1}} \{\mathsf{QComm}(|\psi\rangle) : |\psi\rangle \text{ is a pure state in } \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}, \rho = \mathtt{tr}_{\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |\psi\rangle\langle\psi|\}.$$

On the other hand, suppose $r = \mathsf{QComm}(\rho)$, then Alice, Bob, and Charlie could generate ρ by starting from $\sigma_A \otimes \sigma_B \otimes \sigma_C$, performing local operations and communicating r qubits. For convenience we call this protocol by S. Assume $|\theta_A\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{A_1}$ is a purification of σ_A, and similarly we define $|\theta_B\rangle$ and $|\theta_C\rangle$. We now replace the initial state $\sigma_A \otimes \sigma_B \otimes \sigma_C$ by $|\theta_A\rangle \otimes |\theta_B\rangle \otimes |\theta_C\rangle$ and do the same protocol as S. It can be seen that the output will be a pure state and actually it is a purification of ρ. In this way, we have proved that

$$\mathsf{QComm}(\rho) \geq \min_{\mathcal{H}_{A_1},\mathcal{H}_{B_1},\mathcal{H}_{C_1}} \{\mathsf{QComm}(|\psi\rangle) : |\psi\rangle \text{ is a pure state in } \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}, \rho = \mathtt{tr}_{\mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}} |\psi\rangle\langle\psi|\}.$$

This completes the proof.

The following theorem characterizes the relationship between $\mathsf{QCorr}(\rho)$ and $\mathsf{QComm}(\rho)$ for general multipartite quantum states.

THEOREM 5.4. (Theorem 1.8) *Assume that ρ is a k-partite quantum state in $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_k$. Then*

$$\frac{k}{k-1}\mathsf{QComm}(\rho) \leq \mathsf{QCorr}(\rho) \leq 2\mathsf{QComm}(\rho).$$

Proof. First, we have shown that $\mathsf{QComm}(\rho) \leq \frac{k-1}{k} Q(\rho)$ in Theorem 5.1.

On the other hand, according to Theorem 5.3, we could find a purification $|\psi\rangle$ of ρ in $\mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ such that $\mathsf{QComm}(\rho) = \mathsf{QComm}(|\psi\rangle)$. Then Theorem 5.1 indicates that $\mathsf{QComm}(|\psi\rangle) \geq \frac{1}{2}\mathsf{QCorr}(|\psi\rangle)$. Combing these results with Theorem 4.4, we obtain that

$$\mathsf{QCorr}(\rho) \leq \mathsf{QCorr}(|\psi\rangle) \leq 2\mathsf{QComm}(|\psi\rangle) = 2\mathsf{QComm}(\rho).$$

6 Approximate Quantum Correlation Complexity of Tripartite Pure States

In this section, we prove the results in Subsection 1.4.

THEOREM 6.1. (Theorem 1.9) *Let $|\psi\rangle$ be a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and for an arbitrary small positive number ϵ, let*

$$t_\epsilon(|\psi\rangle) = \lceil \log_2 r_A^{(\epsilon)} \rceil + \lceil \log_2 r_B^{(\epsilon)} \rceil + \lceil \log_2 r_C^{(\epsilon)} \rceil.$$

Then

$$t_\epsilon(|\psi\rangle) \leq \mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle) \leq t_{\epsilon/3}(|\psi\rangle).$$

Proof. Recall that $r_A^{(\epsilon)} = \mathtt{S\text{-}rank}_\epsilon^{(A,BC)}(|\psi\rangle)$, similarly for $r_B^{(\epsilon)}$ and $r_C^{(\epsilon)}$. Suppose $|\phi\rangle$ is a pure state in $\in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ such that $\mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle) = \mathsf{QCorr}(|\phi\rangle)$ and $\mathsf{F}(|\psi\rangle\langle\psi|, |\phi\rangle\langle\phi|) \geq 1 - \epsilon$. Let σ_A is the reduced density matrix of $|\phi\rangle$ in Alice's system, and its rank is s_A; similarly we also define σ_B, s_B, σ_C, and s_C. Look $|\phi\rangle$ as a bipartite pure state with respect to the separation (A, BC), then it holds that $s_A \geq r_A^{(\epsilon)}$, and similarly $s_B \geq r_B^{(\epsilon)}$ and $s_C \geq r_C^{(\epsilon)}$. According to Theorem 4.1, we have that

$$\mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle) = \mathsf{QCorr}(|\phi\rangle) = \lceil \log_2 s_A \rceil + \lceil \log_2 s_B \rceil + \lceil \log_2 s_C \rceil \geq t_\epsilon(|\psi\rangle).$$

On the other hand, Lemma 2.1 shows that $|\psi\rangle$ could be written as

$$|\psi\rangle = \sum_{ijk} a_{ijk} |\alpha_i\rangle|\beta_j\rangle|\gamma_k\rangle,$$

where a_{ijk}'s are complex coefficients, and $\{|\alpha_i\rangle\}$, $\{|\beta_j\rangle\}$, $\{|\gamma_k\rangle\}$ are the nonzero eigenvectors of ρ_A, ρ_B and ρ_C respectively. Without loss of generality, for any $i_1 > i_2$, we suppose $\langle\alpha_{i_1}|\rho_A|\alpha_{i_1}\rangle \geq \langle\alpha_{i_2}|\rho_A|\alpha_{i_2}\rangle$, and $\{|\beta_j\rangle\}$, $\{|\gamma_k\rangle\}$ enjoy the similar orders. We can see that

$$\sum_{i=1}^{r_A}\sum_{j=1}^{r_B}\sum_{k=1}^{r_C} |a_{ijk}|^2 = 1.$$

According to the definition of $r_A^{(\epsilon)}$, we have that

$$\sum_{i=r_A^{(\epsilon/3)}+1}^{r_A}\sum_{j=1}^{r_B}\sum_{k=1}^{r_C} |a_{ijk}|^2 \leq 2\epsilon/3,$$

where we have used Lemma 5.1 of [4] and the fact that

$$\langle\alpha_i|\rho_A|\alpha_i\rangle = \sum_{j=1}^{r_B}\sum_{k=1}^{r_C} |a_{ijk}|^2.$$

Similarly, we have

$$\sum_{i=1}^{r_A}\sum_{j=r_B^{(\epsilon/3)}+1}^{r_B}\sum_{k=1}^{r_C} |a_{ijk}|^2 \leq 2\epsilon/3$$

and

$$\sum_{i=1}^{r_A}\sum_{j=1}^{r_B}\sum_{k=r_C^{(\epsilon/3)}+1}^{r_C} |a_{ijk}|^2 \leq 2\epsilon/3.$$

Thus,

$$\begin{aligned}\sum_{i=1}^{r_A^{(\epsilon/3)}}\sum_{j=1}^{r_B^{(\epsilon/3)}}\sum_{k=1}^{r_C^{(\epsilon/3)}} |a_{ijk}|^2 \geq& 1 - \sum_{i=r_A^{(\epsilon/3)}+1}^{r_A}\sum_{j=1}^{r_B}\sum_{k=1}^{r_C} |a_{ijk}|^2 - \sum_{i=1}^{r_A}\sum_{j=r_B^{(\epsilon/3)}+1}^{r_B}\sum_{k=1}^{r_C} |a_{ijk}|^2 - \sum_{i=1}^{r_A}\sum_{j=1}^{r_B}\sum_{k=r_C^{(\epsilon/3)}+1}^{r_C} |a_{ijk}|^2 \\ \geq& 1 - 2\epsilon.\end{aligned}$$

We now consider a pure state defined as

$$|\phi'\rangle = \frac{1}{\sqrt{m}} \sum_{i=1}^{r_A^{(\epsilon/3)}}\sum_{j=1}^{r_B^{(\epsilon/3)}}\sum_{i=k}^{r_C^{(\epsilon/3)}} a_{ijk}|\alpha_i\rangle|\beta_j\rangle|\gamma_k\rangle,$$

where $m = \sum_{i=1}^{r_A^{(\epsilon/3)}} \sum_{j=1}^{r_B^{(\epsilon/3)}} \sum_{k=1}^{r_C^{(\epsilon/3)}} |a_{ijk}|^2$. It is not difficult to prove that $\mathsf{F}(|\psi\rangle\langle\psi|, |\phi'\rangle\langle\phi'|) \geq \sqrt{1-2\epsilon} \approx 1-\epsilon$. Moreover, according to Theorem 4.1, it holds that $\mathsf{QCorr}(|\phi'\rangle) \leq t_{\epsilon/3}(|\psi\rangle)$. According to the definition of $\mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle)$, we obtain that $\mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle) \leq t_{\epsilon/3}(|\psi\rangle)$.

Actually, following the similar idea that proves the upper bound above, we could get a better one as follows.

Theorem 6.2. *Suppose*

$$R = \min_{S_A,S_B,S_C} \{|S_A| \cdot |S_B| \cdot |S_C| : S_i \subset [r_i] \text{ for i=A,B,C, and } \sum_{i\in S_A}\sum_{j\in S_B}\sum_{k\in S_C} |a_{ijk}|^2 \geq 1-2\varepsilon\}.$$

Then $\mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle) \leq \log_2 \lceil R \rceil$.

The relationship between $\mathsf{QCorr}_\epsilon(|\psi\rangle)$ and $\mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle)$ can be characterized by the following theorem.

Theorem 6.3. (Theorem 1.10) *Let $|\psi\rangle$ be a pure state in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and ϵ is a small positive number. Then*

$$\frac{3}{4}\mathsf{QCorr}_{3\epsilon}^{pure}(|\psi\rangle) \leq \mathsf{QCorr}_\epsilon(|\psi\rangle) \leq \mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle).$$

Proof. Apparently, the definitions indicate that $\mathsf{QCorr}_\epsilon(|\psi\rangle) \leq \mathsf{QCorr}_\epsilon^{pure}(|\psi\rangle)$. For the other direction, according to the definition of $\mathsf{QCorr}_\epsilon(|\psi\rangle)$, there exists a $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$ such that $\mathsf{QCorr}_\epsilon(|\psi\rangle) = \mathsf{QCorr}(\rho)$ and $\mathsf{F}(|\psi\rangle\langle\psi|, \rho) \geq 1-\epsilon$. Then Theorem 4.3 shows that there exists a purification $|\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{A_1} \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_C \otimes \mathcal{H}_{C_1}$ of ρ such that $\mathsf{QCorr}(\rho) \geq \frac{3}{4}\mathsf{QCorr}(|\phi\rangle)$. Thus, we could find a pure state $|\theta\rangle \in \mathcal{H}_{A_1} \otimes \mathcal{H}_{B_1} \otimes \mathcal{H}_{C_1}$ that makes $\mathsf{F}(|\phi\rangle\langle\phi|, |\phi'\rangle\langle\phi'|) \geq 1-\epsilon$, where $|\phi'\rangle = |\psi\rangle \otimes |\theta\rangle$. Recall the definition of $\mathsf{QCorr}_\epsilon^{pure}(|\phi'\rangle)$, and we could obtain that $\mathsf{QCorr}(|\phi\rangle) \geq \mathsf{QCorr}_\epsilon^{pure}(|\phi'\rangle)$. In this way, it holds that $\mathsf{QCorr}(\rho) \geq \frac{3}{4}\mathsf{QCorr}_\epsilon^{pure}(|\phi'\rangle) \geq \frac{3}{4}t_\epsilon(|\phi'\rangle)$, where the last inequality comes from Theorem 6.1. According to Lemma 5.2 of [4], we have that $t_\epsilon(|\phi'\rangle) \geq t_\epsilon(|\psi\rangle)$. Utilizing Theorem 6.1 again, we eventually get that $\mathsf{QCorr}_\epsilon^{pure}(|\phi'\rangle) \geq t_\epsilon(|\psi\rangle) \geq \mathsf{QCorr}_{3\epsilon}^{pure}(|\psi\rangle)$. This means that

$$\mathsf{QCorr}_\epsilon(|\psi\rangle) = \mathsf{QCorr}(\rho) \geq \frac{3}{4}\mathsf{QCorr}_\epsilon^{pure}(|\phi'\rangle) \geq \frac{3}{4}\mathsf{QCorr}_{3\epsilon}^{pure}(|\psi\rangle),$$

and the proof is completed.

Acknowledgments This work is supported by the Singapore Ministry of Education Tier 3 Grant and the Core Grants of the Center for Quantum Technologies, Singapore. Z.W. is also supported in part by the Singapore National Research Foundation under NRF RF Award No. NRF-NRFF2013-13. S.Z. was supported by Research Grants Council of the Hong Kong S.A.R. (Project no. CUHK418710, CUHK419011), and part of the research was done when S.Z. visited Tsinghua University partially supported by China Basic Research Grant 2011CBA00300 (sub-project 2011CBA00301).

References

[1] Andris Ambainis, Leonard Schulman, Amnon Ta-Shma, Umesh Vazirani, and Avi Wigderson. The quantum communication complexity of sampling. *SIAM Journal on Computing*, 32(6):1570–1585, 2003.

[2] Samuel Fiorini, Serge Massar, Sebastian Pokutta, Hans Raj Tiwary, and Ronald de Wolf. Linear vs. semidefinite extended formulations: Exponential separation and strong lower bounds. In *Proceedings of the 44th ACM Symposium on Theory of Computing*, pages 95–106, 2012.

[3] Shengyu Zhang. Quantum strategic game theory. In *Proceedings of the 3rd Innovations in Theoretical Computer Science*, pages 39–59, 2012. Earlier at arXiv:1012.5141 and QIP'11.

[4] Rahul Jain, Yaoyun Shi, Zhaohui Wei and Shengyu Zhang. Efficient protocols for generating bipartite classical distributions and quantum states. *IEEE Transctions on Information Theory*, 59:5171–5178, 2013.

[5] Prahladh Harsha, Rahul Jain, David McAllester, and Jaikumar Radhakrishnan. The communication complexity of correlation. *IEEE Transactions on Information Theory*, 56(1):438–449, 2009.

[6] Michael Nielsen and Isaac Chuang. *Quantum Computation and Quantum Information.* Cambridge University Press, Cambridge, UK, 2000.

[7] Carl Eckart and Gale Young. The approximation of one matrix by another of lower rank. *Psychometrika*, 1(3):211–218, 1936.

[8] Samuel Fiorini, Serge Massar, Sebastian Pokutta, Hans Raj Tiwary, and Ronald de Wolf. Linear vs. semidefinite extended formulations: Exponential separation and strong lower bounds. In *Proceedings of the 44th ACM Symposium on Theory of Computing*, pages 95–106, 2012.

[9] Mihalis Yannakakis. Expressing combinatorial optimization problems by linear programs. In *Proceedings of the 20th Annual ACM Symposium on Theory of Computing*, pages 223–228, 1988.

[10] László Lovász. *Communication complexity: A survey. In book Paths, flows, and VLSI layout edited by B. Korte, L. Lovász, H. J. Prömel, and A. Schrijver.* Springer-Verlag, 1990.

[11] Noam Nisan. Lower bounds for non-commutative computation. In *Proceedings of the 23th Annual ACM Symposium on Theory of Computing*, pages 410–418, 1991.

[12] Moody Chu and Robert Plemmons. Nonnegative matrix factorization and applications. *Linear Algebra and its Applications*, 34:2–7, 2005.

[13] Aaron Wyner. The common information of two dependent random variables. *IEEE Transactions on Information Theory*, 21(2):163–179, 1975.