

Detecting Consistency of Overlapping Quantum Marginals by Separability

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The quantum marginal problem asks whether a set of given density matrices are consistent, i.e., whether they can be the reduced density matrices of a global quantum state. Not many non-trivial analytic necessary (or sufficient) conditions are known for the problem in general. We propose a method to detect consistency of overlapping quantum marginals by considering the separability of some derived states. Our method works well for the k -symmetric extension problem in general, and for the general overlapping marginal problems in some cases. Our work is, in some sense, the converse to the well-known k -symmetric extension criterion for separability.

The quantum marginal problem, also known as the consistency problem, asks for the conditions under which there exists an N -particle density matrix ρ_N whose reduced density matrices (quantum marginals) on the subsets of particles $S_i \subset \{1, 2, \dots, N\}$ equal to the given density matrices ρ_{S_i} for all i [1]. The related problem in fermionic (bosonic) systems is the so-called N -representability problem. It asks whether a k -fermionic (bosonic) density matrix is the reduced density matrix of some N -fermion (boson) state ρ_N . The N -representability problem inherits a long history in quantum chemistry [2, 3].

The quantum marginal problem and the N -representability problem are in general very difficult. They were shown to be the complete problems of the complexity class QMA, even for the relatively simple case where the given marginals are two-particle states [4–6]. In other words, even with the help of a quantum computer, it is very unlikely that the quantum marginal problems can be solved efficiently in the worst case. In this sense, the best hope to have simple analytic conditions for the quantum marginal problem is to find either necessary or sufficient conditions in certain special cases.

When the given marginals are states of non-overlapping subsets of particles, and one is interested in a global *pure* state consistent with the given marginals, both the quantum marginal problem and the N -representability problem were solved [1, 7–11]. However, not much is known for the general problem with overlapping subsystems. For the tripartite case of particles A, B, C , the strong subadditivity of von Neumann entropy enforces non-trivial necessary conditions for the consistency of ρ_{AB} and ρ_{AC} such as $S(AB) + S(AC) \geq S(B) + S(C)$ [12]. In a similar spirit, certain quantitative monogamy of entanglement type of results (see e.g. [13]) also put non-trivial necessary conditions. Necessary and sufficient conditions are generally not known, except in very few special situations [12, 14, 15] when N is small.

In this work, we propose a simple but powerful analytic necessary condition for arguably the simplest overlapping quantum marginal problem, known as the k -symmetric extension problem. That is, we will consider quantum marginal

problems of $k + 1$ particles A, B_1, B_2, \dots, B_k for a given density matrix ρ_{AB} , and require that there is a global quantum state $\rho_{AB_1 B_2 \dots B_k}$ whose marginals on A, B_i equal to the given ρ_{AB} for $i = 1, 2, \dots, k$. The classical analog of this particular case is trivial and there is a consistent global probability distribution as long as the marginals agree on A . In the quantum case, however, the problem remains unsolved even for $k = 2$.

We prove the separability of certain derived state as a necessary condition for the k -symmetric extension problem. A quantum state ρ_{AB} is separable if it can be written as the convex combination $\sum_i p_i \rho_{A,i} \otimes \rho_{B,i}$ for a probability distribution p_i and states $\rho_{A,i}$ and $\rho_{B,i}$. It is now well-known that the k -symmetric extension of ρ_{AB} provides a hierarchy of separability criteria for ρ_{AB} , which converges exactly to the set of separable states when k goes to infinity [16]. This result is essentially given by the quantum de Finetti's theorem [16–21]. Our method can, in some sense, be thought of as a converse to the k -symmetric extension criterion of separability. We will use separability instead as a criterion to test k -symmetric extendability of a bipartite state. This, however, does not cause any circular reasoning problem—we can instead use other known separability criteria, such as the positive partial transpose condition [22, 23], to give necessary conditions for the k -symmetric extension problems.

In particular, our method computes a linear combination $\tilde{\rho}_{AB}^{(k)}$ of the given density matrix ρ_{AB} and its reduced density matrix ρ_A . The separability of $\tilde{\rho}_{AB}^{(k)}$ is then shown to be a necessary condition of the corresponding k -symmetric extension problem for ρ_{AB} .

Interestingly, the condition can also be applied to the more general setting of overlapping quantum marginal problems where the given marginals on A, B_i are different. We reduce them to the k -symmetric extension problems of $\frac{1}{k} \sum_{i=1}^k \rho_{AB_i}$. This averaging method may give trivial conditions in adversarial situations. But it will nevertheless provide non-trivial conditions better than many known results when the given density matrices ρ_{AB_i} , though different, are related in some

way.

Necessary conditions for the k -symmetric extension problems.— Let $\mathcal{H}_A, \mathcal{H}_B$ be two Hilbert spaces of dimension d_A and d_B , respectively. For a Hilbert space \mathcal{H} , let $D(\mathcal{H})$ be the set of density matrices on \mathcal{H} . For a bipartite state $\rho_{AB} \in D(\mathcal{H}_A \otimes \mathcal{H}_B)$, we consider the following overlapping quantum marginal problem: whether there exists a state $\rho_{AB_1 B_2 \dots B_k} \in D(\mathcal{H}_A \otimes (\bigotimes_{i=1}^k \mathcal{H}_{B_i}))$ whose marginals on A, B_i equal to ρ_{AB} for all $i = 1, 2, \dots, k$. The problem is also called the k -symmetric extension problem of ρ_{AB} [16, 24–27] and the global state $\rho_{AB_1 B_2 \dots B_k}$ is called a k -symmetric extension of ρ_{AB} . If such a global state $\rho_{AB_1 B_2 \dots B_k}$ exists, one can choose it to be invariant under permutations of B_1, B_2, \dots, B_k [16, 28].

If the state ρ_{AB} is separable, then it is also obviously k -symmetric extendable for any k . Interestingly, the converse of the statement is also true. That is, if ρ_{AB} is k -symmetric extendable for all k , then ρ_{AB} must be separable [24]. This provides a complete hierarchy of separability criteria. The k -symmetric extension problem can be formulated as a semidefinite programming (SDP), providing a numerical procedure to detect entanglement in a mixed state (see e.g. [29]).

In this paper, we want to know for a given k , whether ρ_{AB} is k -symmetric extendable. One can of course use the semidefinite programming to solve the problem, but the size of the SDP formulation will grow exponentially with k , rendering the approach impractical even numerically for large k . We will instead use the separability of some derived state $\tilde{\rho}_{AB}^{(k)}$ to detect the k -extendability of ρ_{AB} . The important thing is that the dimension of the state $\tilde{\rho}_{AB}^{(k)}$ is independent of k .

For convenience, we will also consider a variant of the k -symmetric extension problem called the k -bosonic extension problem. For Hilbert spaces \mathcal{H}_i of dimension d , let $\bigvee_{i=1}^k \mathcal{H}_i$ be the symmetric subspace of $\bigotimes_{i=1}^k \mathcal{H}_i$. A state ρ_{AB} has a k -bosonic extension if it has a k -symmetric extension $\rho_{AB_1 B_2 \dots B_k}$ whose support on B_1, B_2, \dots, B_k is in the symmetric subspace $\bigvee_{i=1}^k \mathcal{H}_{B_i}$.

Our main observation is the following theorem. In the theorem, \mathcal{H}_A and \mathcal{H}_B are two Hilbert spaces of dimension d_A and d_B respectively.

Theorem 1. *If a bipartite state $\rho_{AB} \in D(\mathcal{H}_A \otimes \mathcal{H}_B)$ has a k -symmetric extension, then the bipartite state*

$$\tilde{\rho}_{AB}^{(k)} = \frac{1}{d_B^2 + k} (d_B \rho_A \otimes I_B + k \rho_{AB}) \quad (1)$$

is separable.

In order to prove this theorem, we first recall the following lemma [30, 31].

Lemma 2. *If a bipartite state $\rho_{AB} \in D(\mathcal{H}_A \otimes \mathcal{H}_B)$ has a k -bosonic extension, then the bipartite state*

$$\hat{\rho}_{AB}^{(k)} = \frac{1}{d_B + k} (\rho_A \otimes I_B + k \rho_{AB}) \quad (2)$$

is separable.

We include a proof of Lemma 2 for completeness, which will directly lead to a proof of Theorem 1 and a generalization to the multi-party marginals case as discussed later.

Proof. Let \mathcal{H}_{B_i} be Hilbert spaces of dimension d_B and let $\rho \in D(\bigvee_{i=1}^k \mathcal{H}_{B_i})$ be a state supported on the symmetric subspace $\bigvee_{i=1}^k \mathcal{H}_{B_i}$. Consider the following superoperator \mathcal{E} :

$$\begin{aligned} \mathcal{E}(\rho) &= \int \langle u |^{\otimes k} \rho | u \rangle^{\otimes k} | u \rangle \langle u | d\mu(u), \\ &= \text{Tr}_{B_1 \dots B_k} \left[(I_B \otimes \rho) \int | u \rangle \langle u |^{\otimes k+1} d\mu(u) \right] \\ &\propto \text{Tr}_{B_1 \dots B_k} \left[(I_B \otimes \rho) \sum_{\pi \in S_{k+1}} W_\pi \right], \end{aligned} \quad (3)$$

where $d\mu(u)$ is the Haar measure over the pure states of \mathcal{H}_B and W_π is the permutation operator defined by

$$W_\pi | i_1, i_2, \dots, i_k \rangle = | i_{\pi^{-1}(1)}, i_{\pi^{-1}(2)}, \dots, i_{\pi^{-1}(k)} \rangle.$$

We claim that

$$\mathcal{E}(\rho) \propto \text{tr}(\rho) I_B + k \rho_B, \quad (4)$$

for all state $\rho \in D(\bigvee_{i=1}^k \mathcal{H}_{B_i})$ where ρ_B is the 1-particle marginal of ρ . The claim follows from the Chiribella's theorem [32]; we give a proof here for its importance to our work. By the fact that any state ρ supported on the symmetric subspace $\bigvee^k \mathcal{H}_B$ can be written as the linear combination of states of the form $|\phi\rangle \langle \phi|^{\otimes k}$ (see the Appendix of [32]), it suffices to prove the claim in Eq. (4) for $\rho = |\phi\rangle \langle \phi|^{\otimes k}$. For all $\pi \in S_k$,

$$\text{Tr}_{B_1 \dots B_k} \left[(I_B \otimes |\phi\rangle \langle \phi|^{\otimes k}) W_\pi \right] = \begin{cases} I_B & \text{if } \pi(1) = 1, \\ |\phi\rangle \langle \phi| & \text{otherwise.} \end{cases}$$

There are $k!$ permutations π such that $\pi(1) = 1$ and $k \cdot k!$ permutations $\pi(1) \neq 1$ and the claim follows from Eq. (3).

If ρ_{AB} has a k -bosonic extension $\rho_{AB_1 B_2 \dots B_k}$, by Eq. (4),

$$\mathcal{I}_A \otimes \mathcal{E}(\rho_{AB_1 B_2 \dots B_k}) \propto \rho_A \otimes I_B + k \rho_{AB}.$$

The separability of $\hat{\rho}_{AB}^{(k)}$ then follows from the positive semidefinite property of $\rho_{AB_1 B_2 \dots B_k}$ and Eq. (3). \square

We now prove Theorem 1.

Proof of Theorem 1. Let $\rho \in D(\mathcal{H}_A \otimes (\bigotimes_{i=1}^k \mathcal{H}_{B_i}))$ be the k -symmetric extension of ρ_{AB} . There exists a purification

$$|\Phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_{A'} \otimes \left[\bigvee_{i=1}^k (\mathcal{H}_{B_i} \otimes \mathcal{H}_{B'_i}) \right]$$

of ρ where $d_{A'} = d_A$ and $d_{B'_i} = d_B$ [33]. State $\sigma = |\Phi\rangle \langle \Phi|$ is the k -bosonic extension of its reduced density matrix $\sigma_{AA' BB'}$ on A, A', B_1, B'_1 . By Lemma 2,

$$\hat{\sigma}_{AA' BB'} = \frac{1}{d_B^2 + k} (\sigma_{AA'} \otimes I_{BB'} + k \sigma_{AA' BB'})$$

is separable between AA' and BB' . Tracing out the systems A' and B' , it follows that

$$\tilde{\rho}_{AB}^{(k)} = \frac{1}{d_B^2 + k} (d_B \rho_A \otimes I_B + k \rho_{AB})$$

is separable. \square

Examples of Bell-diagonal states.— First consider the simple case of $k = 2$, and A, B are qubit systems ($d_A = d_B = 2$). Since for any two-qubit state, the existence of a 2-symmetric extension implies that of a 2-bosonic extension (see Proposition 21 of [28]), we can use the stronger condition of Eq. (2) also for the symmetric extension problem. For simplicity, we will investigate our condition for 2-symmetric extension for the class of Bell-diagonal states. A state ρ_{AB} is Bell-diagonal if it is of the form

$$\rho_{AB} = \sum_{i=1}^4 p_i |\Phi_i\rangle \langle \Phi_i|, \quad (5)$$

where $p_i \in [0, 1]$, $\sum_i p_i = 1$ and

$$\begin{aligned} |\Phi_1\rangle &= (|00\rangle + |11\rangle)/\sqrt{2}, & |\Phi_2\rangle &= (|00\rangle - |11\rangle)/\sqrt{2}, \\ |\Phi_3\rangle &= (|01\rangle + |10\rangle)/\sqrt{2}, & |\Phi_4\rangle &= (|01\rangle - |10\rangle)/\sqrt{2} \end{aligned}$$

are the four Bell states.

A simple computation tells that our condition that $\hat{\rho}_{AB}^{(2)}$ being separable is equivalent to $p_i \in [0, 3/4]$ for all $i = 1, 2, 3, 4$. This is a close approximation of the exact condition of 2-symmetric extendability given in [15, 34–37]:

$$\frac{1}{2} \geq \sum_{i=1}^4 p_i^2 - 4 \left(\prod_{i=1}^4 p_i \right)^{1/2}.$$

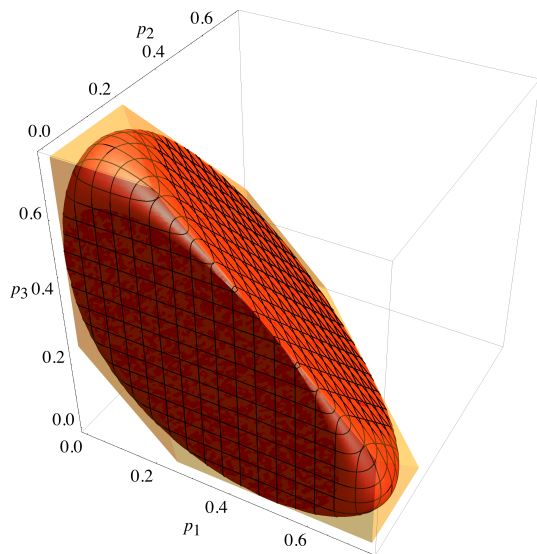
The regions of p_1, p_2, p_3 given by these two conditions are plotted in Fig. 1. The volume of the exact set is approximately 0.15115 and the volume of the polytope given by our condition is 0.15625, which is only about 3% larger.

For comparison purposes, we have also plotted the conditions given by the strong subadditivity (SSA). For Bell-diagonal states, the SSA condition simplifies to $S(AB) \geq 1$. We find that our condition and the SSA condition are incomparable—the non-extendability can sometimes be detected by our condition but not the SSA condition, and vice versa. See Fig. 2 for details.

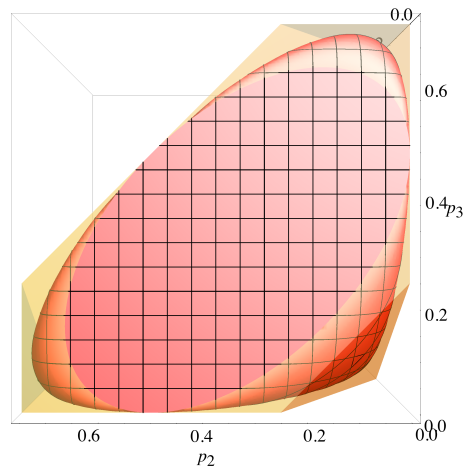
Examples of Werner states.— In our next example, we analyze our conditions for the k -symmetric extension problem of the Werner states [38, 39]. A two-qudit Werner state is a state invariant under the $U \otimes U$ operator for all unitary $U \in \mathbb{U}(d)$ and has the following form

$$\rho_W(\psi^-) = \frac{1 + \psi^-}{2} \rho^+ + \frac{1 - \psi^-}{2} \rho^-,$$

where $\psi^- \in [-1, 1]$ is the parameter, ρ^+ and ρ^- are the states proportional to the projection of the symmetric subspace $\vee^2 \mathbb{C}^d$ and anti-symmetric subspace $\wedge^2 \mathbb{C}^d$ respectively.



(a)



(b)

FIG. 1: (a) The polytope of yellow color characterized by $0 \leq p_i \leq 3/4$ and $1/4 \leq p_1 + p_2 + p_3 \leq 1$ is the condition given by the separability of $\hat{\rho}_{AB}^{(2)}$. The convex set of red color is given by the necessary and sufficient condition for 2-symmetric extension of Bell-diagonal states. (b) is the left view of the same figure.

The Werner state $\rho_W(\psi^-)$ is separable if and only if $\psi^- \geq 0$. The state $\tilde{\rho}_W^{(k)}(\psi^-)$ is separable when $\psi^- \geq -d/k$. Therefore, by Theorem 1, $\rho_W(\psi^-)$ is not k -symmetric extendable if $\psi^- < -d/k$. We note that our bound, though not optimal, is a close approximation of the necessary and sufficient condition $\psi^- \geq -(d-1)/k$ proved in [40] for the k -symmetric extendability of Werner states. This also proves that the k -symmetric extension and k -bosonic extension problems are generally different. In particular, it also implies that the d_B in the linear combination in Eq. (1) is essential for the k -symmetric extension problem.

Applications to the overlapping marginal problems.— We

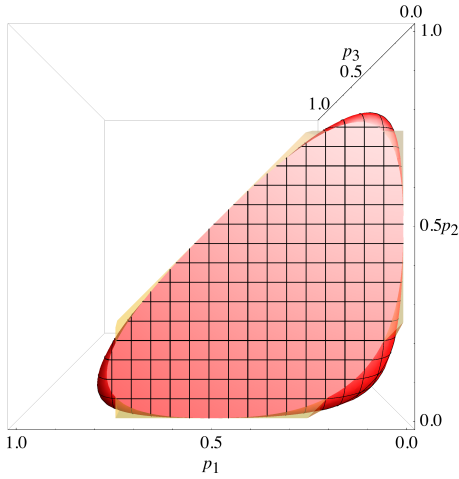


FIG. 2: The two convex sets of (p_1, p_2, p_3) corresponding to the condition given by the separability condition of $\rho_{AB}^{(2)}$ (the polytope of yellow color) and the SSA condition (the convex set of red color).

now extend our method to the more general situation with different marginals on A, B_i . That is, one asks whether there exists a state $\rho_{AB_1B_2\dots B_k} \in D(\mathcal{H}_A \otimes (\bigotimes_{i=1}^k \mathcal{H}_{B_i}))$ whose marginals on A, B_i is the given density matrices ρ_{AB_i} for all $i = 1, 2, \dots, k$. This consistency problem for bipartite marginals is of vital importance in many-body physics and quantum chemistry, where the Hamiltonians of the system in general involve only two-body interactions [2, 3, 41].

In order to use the necessary condition derived in the previous section, we observe the following fact.

Lemma 3. *If the marginals ρ_{AB_i} with $i = 1, 2, \dots, k$ are consistent, then the bipartite state*

$$\rho_{AB} = \frac{1}{k} \sum_{i=1}^k \rho_{AB_i} \quad (6)$$

has k -symmetric extension.

Proof. If ρ_{AB_i} with $i = 1, 2, \dots, k$ are consistent, then there exists a state $\rho_{AB_1B_2\dots B_k} \in D(\mathcal{H}_A \otimes \mathcal{H}_B^{\otimes k})$, such that its reduced density matrix on the system AB_i is ρ_{AB_i} for all $i = 1, 2, \dots, k$. Now consider the state

$$\rho'_{AB_1B_2\dots B_k} = \frac{1}{k!} \sum_{\pi \in S_k} \rho_{AB_{\pi(1)}B_{\pi(2)}\dots B_{\pi(k)}}, \quad (7)$$

where S_k is the symmetric group of k elements. Then $\rho'_{AB_1B_2\dots B_k}$ is a k -symmetric extension of ρ_{AB} . \square

This then allows us to use Theorem 1 and Lemma 2 to detect consistency of bipartite marginals. Consider the example of a three-qubit system with $\rho_{AB} = \rho_W(\psi_1^-)$, and $\rho_{AC} = \rho_W(\psi_2^-)$ for $\psi_i^- \in [-1, 1]$, both of which are two-qubit Werner states. For two-qubit states, 2-symmetric extendability implies 2-bosonic extendability. Hence, we can

use the condition of Eq. (2), which implies that ρ_{AB} and ρ_{AC} are consistent only if $(\psi_1^- + \psi_2^-)/2 \geq -1/2$. This in fact gives a quantitative entanglement monogamy inequality [13, 42–45] for Werner states.

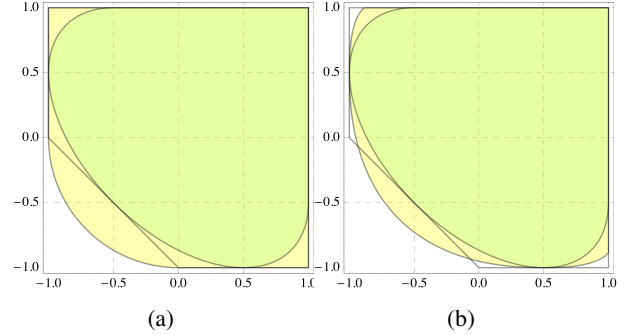


FIG. 3: The green region is the exact condition for two Werner states to be consistent. The pentagon defined by $\psi_1^- + \psi_2^- \geq -1$ and $-1 \leq \psi_i^- \leq 1$ is the condition given by our criterion. (a) is the condition given by the CKW entanglement monogamy inequality, and (b) is the SSA condition.

We compare our condition to that given by the Coffman-Kundu-Wootters (CKW) entanglement monogamy inequality [13],

$$C_{AB}^2 + C_{AC}^2 \leq C_{A(BC)}^2,$$

where $C_{AB} = \max\{0, -\psi_1^-\}$, $C_{AC} = \max\{0, -\psi_2^-\}$ are the concurrences [46, 47] between A, B and A, C respectively, while $C_{A(BC)} = 1$ is the concurrence between subsystems A and BC for Werner states. As shown in Fig. 3a, our condition (the pentagon defined by $\psi_1^- + \psi_2^- \geq -1$ and $-1 \leq \psi_i^- \leq 1$) is always better than the condition given by the CKW inequality (the union of the yellow and green regions).

We have also computed the SSA condition for this particular case and plotted the regions of the SSA condition and our condition in Fig. 3b. Again, the SSA condition (the union of the yellow and green regions) is incomparable with ours.

Generalizations.— Our method extends to the following more general settings. Let $\rho_{AB_1B_2\dots B_r} \in D(\mathcal{H}_A \otimes \mathcal{H}_B^{\otimes r})$ be a given density matrix. The (r, k) -bosonic extension problem of $\rho_{AB_1B_2\dots B_r}$ asks whether there is a global state $\rho_{AB_1B_2\dots B_k} \in D(\mathcal{H}_A \otimes (\bigvee^k \mathcal{H}_B))$ whose marginal on A, B_1, B_2, \dots, B_r is $\rho_{AB_1B_2\dots B_r}$. Following a similar argument as in the proof of Lemma 2 and using the Chiribella's theorem [21, 32], one obtains a necessary condition generalizing Lemma 2. Namely,

$$\hat{\rho}_{AB_1B_2\dots B_r}^{(k)} = \sum_{s=0}^r p_s(k, d_B, r) \mathcal{I}_A \otimes \mathcal{E}_s(\rho_{AB_1\dots B_s}) \quad (8)$$

is an $r + 1$ -party separable state. Here,

$$p_s(k, d, r) = \frac{\binom{k}{s} \binom{d+r-1}{r-s}}{\binom{d+k+r-1}{r}}, \quad (9)$$

is a distribution satisfying $\sum_{s=0}^r p_s = 1$, and \mathcal{E}_s is the super-operator given by

$$\mathcal{E}_s(\rho) = \frac{d_s}{d_r} \Pi_r^+(\rho_s \otimes I^{\otimes(r-s)}) \Pi_r^+, \quad (10)$$

where $d_r = \binom{d+r-1}{r}$, and Π_r^+ is the projection onto the symmetric subspace $\mathcal{V}^r \mathbb{C}^d$.

At the moment, however, we do not know how to generalize the formula in Theorem 1 to this multi-party setting as the procedure of tracing out A', B'_1, \dots, B'_r does not commute with the projection Π_r^+ in general. We leave it as an open problem for future work.

Summary and discussion.— We have proposed a method to detect consistency of overlapping quantum marginals. The key idea is to construct some other density matrix from the linear combinations of the local density matrices and test the separability of the derived density matrix. Our idea is closely related to the finite quantum de Finetti's theorem [16, 19, 20, 48], which states that the r -particle marginal of a symmetric N -particle state cannot be too far from an r -particle separable state, with a distance bounded by $O(1/N)$ for fixed d and r . Therefore, if an r -particle state is too far from a separable state, then it cannot be the marginal of a symmetric N -particle state. However, to directly check the distance to the nearest separable state is not easy. Moreover, the bound given in the known versions of finite quantum de Finetti's theorem are in general not tight, so when N is small those bound may not be useful.

For comparison, our method gives simple necessarily conditions, which are evidently good even for N small. Our method can also lead to improved bound in the finite de Finetti's theorem. For instance, as a direct consequence of Theorem 1, we can obtain that for any k -symmetric extendible state ρ_{AB} , its distance to separable states is upper bounded by

$$\min_{\rho \in \text{Sep}} \|\rho_{AB} - \rho\|_1 \leq \left\| \rho_{AB} - \tilde{\rho}_{AB}^{(k)} \right\|_1 \leq \frac{2d_B^2}{d_B^2 + k}, \quad (11)$$

which slightly improves that of [20].

Another direct application is that in Lemma 2 if we choose $k = 1$, then from Eq. (2), we get that for any bipartite state ρ_{AB} , the state

$$\sigma_{AB} = \frac{1}{d_B + 1} (\rho_A \otimes I_B + \rho_{AB}), \quad (12)$$

is always separable. Notice that Eq. (12) implies that $\sigma_A = \rho_A$, so we have $(d_B + 1)\sigma_{AB} - \sigma_A \otimes I_B = \rho_{AB} \geq 0$. This gives an interesting sufficient condition of separability for σ_{AB} : if $(d_B + 1)\sigma_{AB} \geq \sigma_A \otimes I_B$, then σ_{AB} is separable. We may also compare this with the known necessary condition of separability for σ_{AB} [49, 50]: if σ_{AB} is separable, then $\sigma_{AB} \leq \sigma_A \otimes I_B$.

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of this fact follows along similar lines of Lemma 22.1 (Lecture 22).

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