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Quantifying quantum information resources: a numerical study

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Abstract Quantum systems present correlations, which cannot be offered by classical objects. These distinctive correlations are not only considered as fundamental features of quantum mechanics, but more importantly, they are regarded as critical resources for different quantum information tasks. For example, quantum entanglement has been established as the key resource for quantum communication, and quantum discord has been suggested as the resource in deterministic quantum computation with one qubit (DQC1). However, quantification of these resources is very difficult, especially for many-body situations. Here, we introduce a unified numerical method to quantify these resources in general multiqubit states and use it to investigate the robustness of quantum discord in multiqubit permutation-invariant states. Our method paves the way to quantitatively investigate the relation between the potential of quantum technologies and quantum resources, particularly, that between quantum computation and quantum correlations.

Keywords quantum, quantum information, quantum computation, entanglement, quantum discord, numerical algorithm, replica exchange Monte Carlo

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1 Introduction

Quantum correlations, which cannot be observed in classical systems, are regarded as the characteristic features of quantum mechanics. More importantly, these correlations are widely considered as resources for certain quantum tasks. Entanglement, which characterizes the non-local property of quantum states, has been established as the core of quantum information science and a crucial resource for quantum communication and quantum key distribution [1–3]. It is widely believed that entanglement is also the key resource for quantum computation. However, in the deterministic quantum computation with one pure qubit (DQC1) protocol [4, 5], there is no entanglement in the system and DQC1 is more efficient than classical computing. Thus, another quantum correlation, quantum discord, which is different from entanglement and was initially introduced by Ollivier and Zurek [6], is proposed as the resource for DQC1. Recently, quantum Bell-Kochen-Specker contextuality [7,8], which is another property of quantum

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mechanics, has been proved as the resource for universal quantum computation through magic distillation [9, 10].

Since these quantum correlations act as advantageous resources for quantum tasks, it is very important to understand the potential of these resources, and the first step to achieve this is to quantify the resources. Various methods have been introduced to quantify quantum correlations; for example, quantum concurrence [11], quantum entropy [12], distillation entanglement [13, 14] and tangle [15] have been introduced to quantify entanglement in quantum states. Different methods have also been introduced to measure quantum discord [16–19]. Quantification of quantum contextuality has also been recently introduced in [20]. Given the richness of definitions for various quantum resources, there are still two issues worth noting. First, the subtle differences between different measurements have made it impossible to compare one type of resource to another. Second, from the numerical aspect, measurements of the resources are usually very difficult, especially, for general many-body systems.

According to the unified resource theory [21], we can divide all quantum resources into two sets: one set is considered free where the measurement of the corresponding resource is zero, and the other is considered valuable. Unified quantification of the resources has been proposed by Modi et al. [19] by using relative entropy as a measure of the distance between the concerned state and the free resource. While this measurement considers all resources on an equal footing, it also requires minimization of the distance between the target state and the free resource, to which a general analytical solution remains unknown.

To solve this minimization problem, in this work, we develop a reliable and efficient numerical method based on replica exchange Monte Carlo (also known as parallel tempering algorithm) [22–25] for calculating these resources of arbitrary multiqubit states by using the definition of relative entropy. We then verify our method by comparing the numerical results with analytical solutions of some well-known states. Finally, we apply our method to investigate the robustness of quantum discord in the bit-flipping process of multiqubit permutation-invariant states, which could not be solved analytically in general.

2 Geometry of correlations

From a geometric point of view, the value of a desired property in a quantum state can be quantified by the distance between itself and its closest state without that desired property, i.e., in the free resource set [19]. For example, quantum entanglement E can be defined by the distance between an entangled state and its closest separable state where the entanglement is zero. When the distance is measured in terms of the relative entropy, it is known as the relative entropy of entanglement [26], which can be written as

$$E = \min_{\sigma \in \mathcal{S}} S(\rho \| \sigma)\,, \tag{1}$$

where $\mathcal{S}$ is the set of all separable states, i.e. states of the form $\sigma = \sum_i p_i \pi_1^i \otimes \cdots \otimes \pi_N^i$, where π_n, with $n = 1, 2, \ldots, N$, is the state of the nth subsystem. $S(\rho\|\sigma) = \mathrm{tr}\left(\rho \log \frac{\rho}{\sigma}\right) = \mathrm{tr}\left(\rho \log \rho\right) - \mathrm{tr}\left(\rho \log \sigma\right)$, represents the relative entropy between the entangled state ρ and separable state σ.

In the same way, the quantum discord D can be defined as the distance between an entangled state ρ and its closest classical state χ where discord is zero, i.e.,

$$D = \min_{\chi \in \mathcal{C}} S(\rho \| \chi)\,. \tag{2}$$

$\mathcal{C}$ is the set of all classical states, which have the form of

$$\chi = \sum_{k_1 \ldots k_N} p_{k_1 \ldots k_N} |k_1 \ldots k_N\rangle\langle k_1 \ldots k_N|\,, \tag{3}$$

where $|k_n\rangle$, with $n = 1, 2, \ldots, N$, is the local orthonormal base for the nth subsystem.

In this work, we use the above definitions (same as in [19]) for entanglement and quantum discord. Clearly, all definitions require finding the minimum in a set of states, which is generally difficult when the

Hilbert space of states is large. This minimization problem can become even harder for quantum discord, since the set of classical state $\mathcal{C}$ is not convex [19] and the traditional convex optimization methods fail in such situations. In the following section, we introduce a general numerical method that can be used to calculate correlations for arbitrary multiqubit systems. The method can be easily generalized for multipartite systems consisting of qutrits or qudits.

3 Numerical method

The key problem of quantifying quantum correlations based on distance is to determine the closest state in the free resource set, which could be transformed into a general constrained global minimization problem. For entanglement, the global minimum of the "target function" (energy function) is searched in the space of all separable states. To parameterize the search, we can rewrite an N-partite separable state as a composition of N_p pure states, i.e.,

$$x_s = \sum_{j=1}^{N_p} p_j |\psi_1^j \dots \psi_N^j\rangle\langle\psi_1^j \dots \psi_N^j| \,, \tag{4}$$

where $|\psi_n^j\rangle\,(j = 1, \dots, N_p, n = 1, \dots, N)$ is an arbitrary qubit represented by two variables θ_n^j and ϕ_n^j in the form $|\psi_n^j\rangle = \cos\theta_n^j|0\rangle + \mathrm{e}^{\mathrm{i}\phi_n^j}\sin\theta_n^j|1\rangle$ with $\theta_n^j \in [0, \pi]$ and $\phi_n^j \in [0, 2\pi]$. According to Caratheodory's theorem, the number of composition N_p is at most $[\dim(H_1) \times \dim(H_2) \times \cdots \times \dim(H_N)]^2$, where $\dim(H_n)$ is the Hamiltonian dimension of the nth subsystem, and the maximum N_p is 2^{2N} for multiqubit systems. As a result, the problem becomes a minimization in the target searching space of $N_v = N_p + 2N_pN$ variables with two constraints, where N_v is defined as the total number of variables. The first constraint is the normalization condition $\sum_j p_j = 1$ with $p_j \geqslant 0$, and the second is the available ranges for variables θ_n^j and ϕ_n^j; these constraints are enforced by applying the normalization factor on p_j and cyclic boundary conditions on θ_n^j and ϕ_n^j at each Monte Carlo (MC) step accordingly. Finally, the target function for entanglement T_e is defined as the relative entropy between a given state y and the separable state x_s to be minimized, i.e.,

$$T_e(\{p_j, \theta_n^j, \phi_n^j\}) = S(y\|x_s(\{p_j, \theta_n^j, \phi_n^j\}))\,. \tag{5}$$

When calculating the relative entropy of quantum discord, the global minimum should be located in classical states. Eq. (3) above shows that the classical state can be written as a mixture of locally distinguishable states, which consist of local orthonormal bases. So, in order to produce an arbitrary classical state, we first generate an arbitrary local orthonormal basis by applying a general unitary transformation

$$U(\theta, \phi) = \begin{bmatrix} \cos\theta & \sin\theta\mathrm{e}^{\mathrm{i}\phi} \\ -\sin\theta\mathrm{e}^{-\mathrm{i}\phi} & \cos\theta \end{bmatrix} \tag{6}$$

on the simplest local orthonormal basis, which is the computational basis of a qubit, i.e. $\{|0\rangle, |1\rangle\}$. As a result, an arbitrary orthonormal basis of the nth qubit can be written as

$$\{|k_n\rangle\} = \{\cos\theta_n|0\rangle + \sin\theta_n\mathrm{e}^{\mathrm{i}\phi_n}|1\rangle, -\sin\theta_n\mathrm{e}^{-\mathrm{i}\phi_n}|0\rangle + \cos\theta_n|1\rangle\}\,. \tag{7}$$

Following (3), an arbitrary classical state is obtained as the direct product of the generated bases, i.e.,

$$x_c = \sum_{j=1}^{N_b} p_j(|k_1\rangle \otimes \cdots \otimes |k_N\rangle)(\langle k_1| \otimes \cdots \otimes \langle k_N|). \tag{8}$$

Since description of each qubit needs two variables θ_n and ϕ_n, we need $N_v = N_b + 2N$ variables in total to represent the state, and for an N-qubit system, $N_b = 2^N$. The constraints for p_j, θ_n and ϕ_n are the same as those for entanglement, and the target function for discord T_d is represented as

$$T_d(\{p_j, \theta_n, \phi_n\}) = S(y\|x_c(\{p_j, \theta_n, \phi_n\}))\,, \tag{9}$$

where y is the given state and x_c is the classical state to be minimized.

Taking a 4-qubit system as an example, the number of variables in the target functions of entanglement and quantum discord are 2304 and 24, respectively. For systems with more qubits, the number of variables can be very large, especially for entanglement. The "energy" surface of the target functions, therefore, could be very complex and may have numerous local minima. To obtain a reliable global minimum, we adopt the replica exchange Monte Carlo method [22–25], which has been successfully applied in condensed matter physics to solve many complex minimization problems, such as spin glasses [27] and Lennard-Jones particles [28, 29] and more recently in quantum realm to solve three-tangle [30], to minimize the target functions. Instead of taking MC steps while cooling down the system like in the conventional simulated annealing algorithm, this method simulates N_r replicas of the system simultaneously, each at a different temperature $\beta_0 = 1/T_{\max} < \beta_1 < \cdots < \beta_{M-2} < \beta_{M-1} = 1/T_{\min}$, covering a range of interest. Each replica runs independently, except that after certain steps, the configurations can be exchanged between neighboring temperatures according to the Metropolis criterion,

$$w = \begin{cases} 1, & \Delta H < 0, \\ \mathrm{e}^{-\Delta H}, & \text{otherwise.} \end{cases} \tag{10}$$

To satisfy the detailed balance in canonical ensemble, ΔH is set to be $\Delta H = -(\beta_i - \beta_{i-1})(E_i - E_{i-1})$, in which E_i and E_{i-1} are the energy of the ith and $(i-1)$th replica. While the replicas with lower temperatures are good at discovering the local minima, replicas with higher temperatures are able to cover a wider range of the "energy" landscape. The inclusion of high-T configurations ensures that the low-T systems can access a broad searching space and avoid becoming trapped at the local minima. In our calculations, the temperature range is chosen to be $T_{\max} = 100$ and $T_{\min} = 10^{-6}$, which gives the minimized value an accuracy of 10^{-6} theoretically. With the given range of temperature, the number of replicas is chosen to be around 80, which is sufficient to allow a reasonable exchange between replicas and to solve the target functions in the scope of this work. The intervals between neighboring temperatures are adjusted to ensure that the acceptance rate of configuration exchange stays around 20%, which is an optimal rate from our experience. For clarity, we sum up the main process of the algorithm as three nesting recursions.

- Outer Loop : For each n_1 temperature exchange, adjust temperature intervals once.
- Middle Loop : For each n_2 MC steps, exchange configurations between neighboring replicas once.
- Inner Loop : All replicas take regular MC steps and update the minimum value of target function.

With simple adjustments to the definition of searching space, this method could be generalized to systems with qutrits, qudits or even more complex subsystems. For example, a general N-qutrit separable state could be defined as in (4), only here $|\psi_n^j\rangle$ is a qutrit defined by three variables $\alpha_n^j, \beta_n^j, \gamma_n^j$ as $|\psi_n^j\rangle = \alpha_n^j|0\rangle + \beta_n^j|1\rangle + \gamma_n^j|2\rangle$ which satisfies the normalization constraint $|\alpha_n^j|^2 + |\beta_n^j|^2 + |\gamma_n^j|^2 = 1$. The normalization condition on p_j remains the same. Note that the maximum N_p for a N-qutrit system is 3^{2N}, and the set of separable state is a searching space of $N_v = N_p + 3N_pN$ variables with two constraints. The target function for entanglement is defined as

$$T_e(\{p_j, \alpha_n^j, \beta_n^j, \gamma_n^j\}) = S(y \| x_s(\{p_j, \alpha_n^j, \beta_n^j, \gamma_n^j\}))\,, \tag{11}$$

where x_s represents the N-qutrit separable state and the relative entropy of entanglement for a multi-qutrit system can be computed with the same minimization process. A d-level quantum system (qudit) could be described by d variables and the generalization could follow the same procedure, resulting in a minimization problem for a searching space of $N_v = N_p + dN_pN$ variables. However, in this work, we will restrict the discussion within multiqubit systems.

Replica exchange Monte Carlo is well known for its higher efficiency in finding global minimum compared to traditional methods such as simulated annealing. For multiqubit systems with up to 6 qubits studied in this work, the computation does not take more than a few hours on a cluster computer with CPUs at 2.67 GHz. However, for general multipartite systems, the computational complexity of the algorithm is related to the number of variables N_v in the searching space and the number of replicas N_r. It is

widely agreed [31–33] that for a general minimization problem, the time needed for simulated annealing to hit the minimum has a polynomial dependence on the number of variables, namely $O(N_v^m)$, where m a nonnegative integer. replica exchange Monte Carlo, which can be seen as a paralleled version of simulated annealing, multiplies the time complexity with the number of replicas N_r and reads $O(N_r N_v^m)$. For example, for solving N-qudit entanglement, the time complexity would be $O(N_r(N_p + dN_pN)^m)$. While it seems that the parallel algorithm with N_r replicas cost N_r times of CPU resources needed for a single-threaded simulated annealing, comparisons [34–36] have shown that the replica exchange algorithm offers a higher possibility of finding the global minimum than N_r times run of simulated annealing, since the latter is more often trapped in the local minima. In total, the replica exchange algorithm offers a shorter waiting time to solve the minimization problem. The memory cost of the algorithm grows linearly with the number of variables and the number of replicas used, i.e., $O(N_r N_v)$. Because of the parallel nature of the method, only $O(N_v)$ memory is needed for each CPU in the cluster computer. In a word, the time and space complexity of the algorithm are both manageable with a general cluster computer setup.

4 Verification of numerical method

To test our method, we first calculate the entanglement for a mixture of permutation-invariant states [37] as

$$\rho_{n;k_1,k_2}(\alpha) \equiv \alpha|S(n,k_1)\rangle\langle S(n,k_1)| + (1-\alpha)|S(n,k_2)\rangle\langle S(n,k_2)|\,, \tag{12}$$

where

$$|S(n,k)\rangle = \frac{\sqrt{C_k^n}}{n!}\sum_i \Pi_i|\underbrace{0\cdots0}_{k}\underbrace{1\cdots1}_{n-k}\rangle. \tag{13}$$

For a 4-qubit system, we calculate the state

$$\rho_{4;3,1}(\alpha) = \alpha|S(4,1)\rangle\langle S(4,1)| + (1-\alpha)|S(4,3)\rangle\langle S(4,3)|\,, \tag{14}$$

for which Wei et al. [37] have provided the analytical results. Our numerical results are compared to the analytical results in Figure 1. We see that the numerical and analytical results agree perfectly with each other, with error $\sim 10^{-4}$.

For quantum discord, we compare our results for arbitrary superposition of two canonical orthonormal GHZ states [38], i.e.,

$$|G_{02}\rangle = \cos\alpha|G_0^+\rangle + \sin\alpha e^{i\gamma}|G_2^+\rangle\,, \tag{15}$$

where

$$|G_i^+\rangle = \frac{|B_N(i)\rangle + |B_N(2^N-1-i)\rangle}{\sqrt{2}}\,, \tag{16}$$

in which $i = 0, 1, \ldots, 2^{N-1}$ and $|B_N(i)\rangle$ represents the binary string converted from the decimal number i. Analytical solutions for quantum discord of such states were obtained by Parashar et al. [38]. According to their results, quantum discord for 4 and more qubit states have the same expression as follows, regardless of γ,

$$D = -c^2\log_2(c^2/2) - (1-c^2)\log_2((1-c^2)/2)\,, \tag{17}$$

where $c = \cos\alpha$, $s = \sin\alpha$. We numerically calculate the quantum discord of 4 and 5-qubit systems with $\gamma = 0$, and compare them with the analytical results in Figure 2, from which we can see that the numerical results agree well with the analytical results.

We also calculate the entanglement and quantum discord of W state and cluster state. To demonstrate the accuracy, the results are listed in Table 1. Numerical results are in excellent agreement with the analytical ones provided by Modi et al. in [19], with a general accuracy of 10^{-4}. In a word, our numerical methods are reliable in measuring these two types of quantum resources.

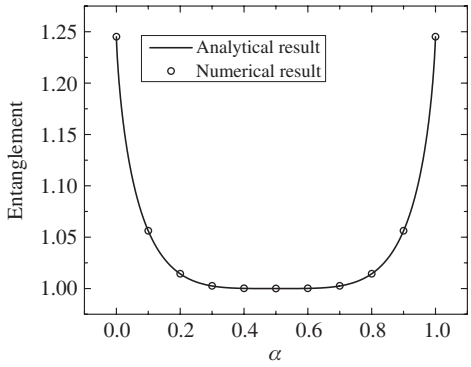

Figure 1 Entanglement of 4-qubit permutation-invariant state, i.e., Eq. (14) mixed by $|S(4,1)\rangle$ and $|S(4,3)\rangle$. The analytical result is represented by solid line and the numerical result by open circles.

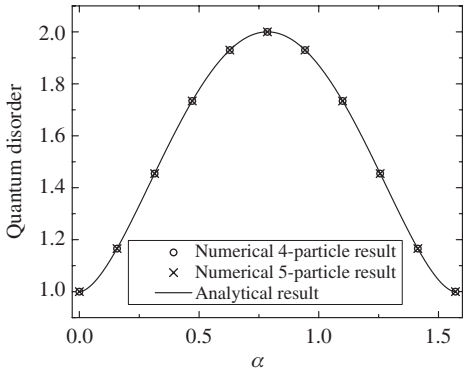

Figure 2 Quantum discord of 4 and 5-qubit superpositions of two canonical orthonormal GHZ states as in (15). The 4-qubit numerical result is represented by open circles and the 5-qubit numerical result by crosses, compared to the analytical result represented by solid line.

Table 1 Numerical versus analytical results for 3-qubit W state and 4-qubit cluster state

W state	Entanglement	Quantum discord
Modi et al.	1.169925001	~ 1.58
Numerical results	1.169948999	1.584962851
Cluster state	Entanglement	Quantum discord
Modi et al.	2	2
Numerical results	2.000139316	2.000002430

5 Quantum discord of multiqubit permutation-invariant states

The robustness of entanglement and discord in quantum manipulation process is critical for quantum algorithms based on these two types of resources. While previous results have shown that entanglement experiences "sudden death" [39] when the system interacted with environment, it has been suggested that discord could be much more robust in the same decoherence process [40]. Here, with the confidence of our numerical method, we investigate the robustness of quantum discord of multiqubit permutation-invariant states in the bit-flipping process, for which previous results on entanglement has been reported in [37].

A general mixture of permutation-invariant states is defined as

$$\rho = \alpha|S(n,1)\rangle\langle S(n,1)| + (1-\alpha)|S(n,n-1)\rangle\langle S(n,n-1)|\,, \tag{18}$$

where α ranges from 0 to 1. If we take $|S(n,n-1)\rangle$ as the initial state and $|S(n,1)\rangle$ as the final state, and noting that $|S(n,1)\rangle$ and $|S(n,n-1)\rangle$ are connected through bit-flipping operations, the variation of α from 0 to 1 can be thought as a certain kind of collective bit-flipping process.

Figure 3 depicts the change of quantum discord with α for $N = 3-6$ qubits. As expected, quantum discord is generally larger for a larger system. Remarkably, while the quantum discord of 3 qubit state varies, the quantum discord of 4 to 6 qubits stays "frozen" when α goes from 0 to 1. This is interesting because it suggests that for these multiqubit states, the quantum discord is not affected by certain collective operations. The dynamics of quantum discord is drastically different from that of entanglement, since according to Wei et al. [37], entanglement varies through the same bit-flipping process in such systems. Therefore, our results show that quantum discord surpasses entanglement in stability.

We then add another permutation-invariant state $|S(4,2)\rangle$ to the 4-qubit state mentioned above and form the following mixed state,

$$\rho = \alpha(1-\beta)|S(4,1)\rangle\langle S(4,1)| + \beta|S(4,2)\rangle\langle S(4,2)| + (1-\alpha)(1-\beta)|S(4,3)\rangle\langle S(4,3)|\,, \tag{19}$$

where α, $\beta \in [0,\,1]$. The quantum discord of this state is plotted in the α-β plane in Figure 4. When

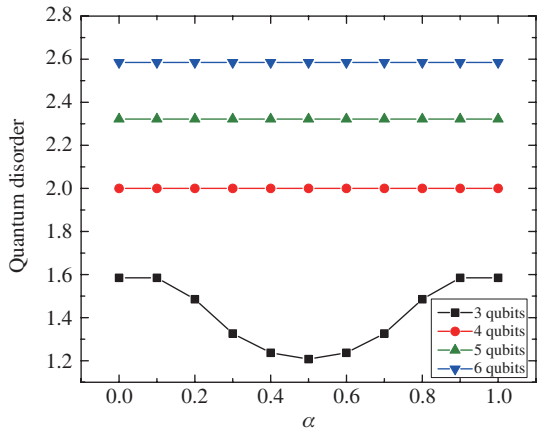

Figure 3 (Color online) Quantum discord of 3 to 6 qubit states (18) mixed by permutation-invariant states $|S(n,1)\rangle$ and $|S(n,n-1)\rangle$.

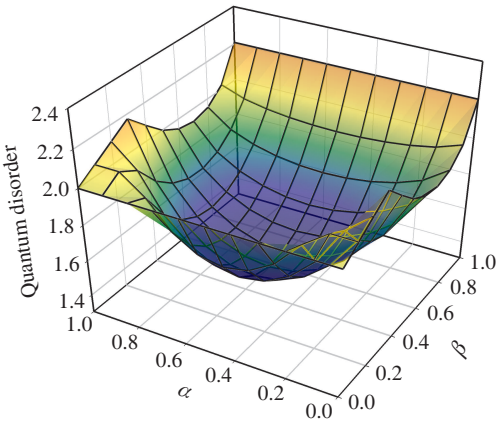

Figure 4 (Color online) Quantum discord of 4-qubit states (19) mixed by $|S(4,1)\rangle$, $|S(4,2)\rangle$ and $|S(4,3)\rangle$, plotted on α-β plane.

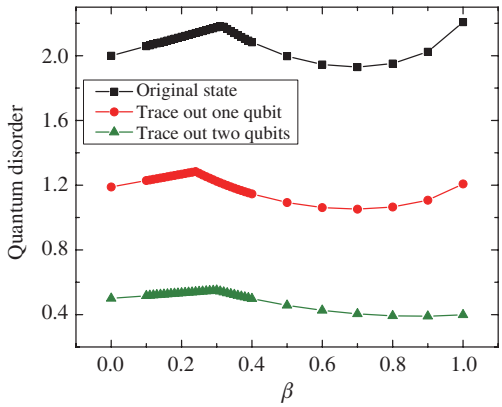

Figure 5 (Color online) Robustness of the turning point: Quantum discord of the original 4-qubit state in (19) when $\alpha = 0$, and the states after tracing out one and two qubits from the original state. The turning point exists in all three states, showing its robustness.

$\beta = 0$, this state reduces to the state given in (18), and the quantum discord stays frozen with the change of α. However, when β is non-zero, the quantum discord does not remain constant, as shown in Figure 4. This suggests that the "frozen quantum discord" property is strongly dependent on the form of the states. Therefore, if one wants to harness the stability of the quantum discord of a multipartite system, the initial state must be carefully chosen.

In the cases of $\alpha = 0$ or 1, i.e. in absence of the $|S(4,1)\rangle$ or $|S(4,3)\rangle$ state, a sudden change occurs in the quantum discord at $\beta = 0.31$. We investigate the robustness of the turning point by fixing $\alpha = 0$, and tracing one and two qubits out of the system. As shown in Figure 5, the turning point of quantum discord still exists after tracing out one and two qubits, demonstrating its robustness. The position of the turning point shifts to ~ 0.24 on tracing out one qubit, and change back to ~ 0.3 on tracing out two qubits. The reason for this phenomenon is interesting for future investigation.

6 Conclusion

We have developed a reliable and efficient numerical method to calculate different types of quantum resources based on the relative entropy of an arbitrary multiqubit state. We have verified the methods for different states with entanglement and discord. All numerical results agree extremely well with existing

analytical solutions, which validates our numerical method. We also demonstrate for the first time "frozen quantum discord" and other interesting phenomena in multiqubit systems and show that quantum discord can be more robust than entanglement in bit-flipping process. We note that with very straightforward modifications to the searching space of the target set of states, the method introduced here can be directly extended to quantify multipartite systems consisting of qutrits or qudits. Our numerical method paves the way to quantitatively investigate the resources in quantum tasks and further determine the relation between the resources and the potential of quantum technologies.

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Conflict of interest The authors declare that they have no conflict of interest.

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