Upper bounds for relative entropy of entanglement based on convex hull approximation

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Quantifying entanglement for multipartite quantum state is a crucial task in many aspects of quantum information theory. Among all the entanglement measures, relative entropy of entanglement $E_R$ is an important quantity due to its clear geometric meaning, easy compatibility with different system sizes, and various applications in many other related quantity calculations. Lower bounds of $E_R$ were previously found based on distance to the set of positive partial transpose states. We propose a method to calculate upper bounds of $E_R$ based on the convex hull approximation of the set of separable states. We apply our method to calculate $E_R$ for composite systems of various sizes, and compare with the previous known lower bounds, obtaining promising results. Our method adds a new tool for entanglement measure calculation and deepens our understanding for the structure of separable states.

I. INTRODUCTION

Quantum entanglement is a kind of correlation that is beyond any possible classical probabilistic correlation [1]. Entanglement has played a crucial role in almost all aspects of quantum information theory, such as quantum channel capacity [2], quantum algorithm [3], quantum error correction [4] and quantum sensing [5]. In recent years, entanglement also becomes a central concept in the interdisciplinary field of quantum information theory, condensed matter physics, and quantum gravity [6, 7].

For any given (multipartite) quantum state $\rho$, one fundamental question one would like to know is whether $\rho$ is entangled or not, and a further question, how much $\rho$ is entangled [8]. Entanglement measures are quantities providing such kind of information. Normally, an entanglement measure $E(\rho)$ satisfies some natural assumptions such as invariance under local unitary operations, and non-increasing under general local operations [9, 10].

Among many entanglement measures, relative entropy of entanglement $E_R$ is one important quantity [11]. For any quantum state $\rho$, $E_R(\rho)$ naturally measures “how far” $\rho$ is from the set of separable states. As illustrated in Fig. 1, inside the quantum state space, for an entanglement state, which is represented by $A$ or $B$, the relative entropy of entanglement is the distance of the state to the set of separable state (denoted by SEP in the figure). Or equivalently, the task of finding $E_R(\rho)$ is to look for a state in SEP ($A'$ or $B'$) to minimize distance to the entangled state $\rho$ ($A$ or $B$). Besides having a good geometric interpretation, $E_R(\rho)$ is also known to be compatible for multiparty systems, providing an upper bound for entanglement distillation [12, 13], and connected to the study of many other aspects in quantum information theory, such as the use of relative entropy in some information-theoretic quantities [11, 14].

Calculation of $E_R(\rho)$ is an optimization problem over

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the set of separable states [15]. Such a set of separable states is notoriously hard to characterize, despite known to be convex [1]. On the other hand, the set of states with positive partial transpose (PPT) is much easier to characterize [16]. Calculating “how far” the state $\rho$ is from the set of PPT states in terms of relative entropy can then be formulated as a certain kind of Semi-Definite Programming (SDP) [17, 18]. This then gives a lower bound of $E_R(\rho)$, as illustrated in Fig. 1. As we know, the set of separable states (SEP in Fig 1) is a subset of the set of PPT states (PPT in Fig 1). Therefore, for some states, such as the state $B$, the closest state in PPT is $B''$, while the closest state in SEP is $B'$. Consequently, the distance of $BB'$ is smaller than $BB''$, hence the point $B''$ gives a lower bound for $E_R(\rho)$.

In this work, we propose a method to calculate upper bounds for $E_R(\rho)$. Our idea is based on the convex hull approximation (CHA) of the set of separable states [19]. Notice that the extreme points of the set of separable states, which is convex, are simply pure product states. CHA is then the convex hull of a large number of randomly generated extreme points, which approximates the convex set from inside. The “distance” from $\rho$ to CHA in terms of relative entropy then gives a upper bound of $E_R(\rho)$. As illustrated in Fig. 2, the idea is to generate the extreme points of the set SEP ($\{\sigma_i\}$), then form a convex hull of $\{\sigma_i\}$, giving a CHA for SEP. Over this CHA, we can find a state $\sigma$, which minimizes the distance of $\sigma$ to $\rho$. Obviously, the state $\sigma$ gives an upper bound of $E_R(\rho)$. In case the set of extreme points are chosen properly, the relative entropy of entanglement could be very close to the true value.

We apply our method to calculate $E_R(\rho)$ for composite systems of various sizes, and compare our results with the previous lower bounds given by SDP. We consider bipartite system of dimension $d_A \otimes d_B$. In the case of $d_A d_B \leq 6$, where the set of PPT is the same as that of SEP [16], our results are very close to the former results based on PPT. In the case of $d_A d_B > 6$, our method gives an upper bound, which is always larger that the value given by PPT, and in many cases we believe that our value is more close to the actual value of $E_R(\rho)$. Our results add a new tool for entanglement measure calculation and deepen our understanding about the difference between the set structures of SEP and PPT.

We organize our paper as follows: in Sec II, we discuss our algorithm based on CHA. In Sec III, we show our results in different situations: firstly for two kinds of states (Werner states and isotropic states), for which we know the analytical form of their relative entropy of entanglement, to compare and check the validity of our algorithm; secondly for a special case of states that are bound entangled (i.e. entangled state that are PPT), we calculate their relative entropy of entanglement, to demonstrate that our method gives better estimation for the true value of than the method of PPT; finally for different dimensions, we generate random states and calculate their relative entropy of entanglement, to demonstrate the power of our method for giving new understandings of the difference between SEP and PPT. In Sec IV, we summarize our results and discuss some future directions.

## II. ALGORITHM

In this section, we discuss our algorithm for calculating the upper bounds of relative entropy of entanglement based on CHA.

For a given bipartite system $AB$ with Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, a state $\rho_{AB}$ is separable if it can be written in a convex combination

$$\rho_{AB} = \sum_i A_i \rho_A^{(i)} \otimes \rho_B^{(i)},$$

(2.1)

where $\rho_A$ and $\rho_B$ are states in Hilbert space $\mathcal{H}_A$ and $\mathcal{H}_B$, respectively. The set of all separable states, denoted by SEP, is a convex set, given by its definition. The extreme points of SEP is given by the states of the form $\rho_A \otimes \rho_B$, where $\rho_A$ and $\rho_B$ are arbitrary pure states.

Denote the convex set of SEP as $D$. For any given bipartite state $\rho$, the relative entropy of entanglement $E_R(\rho)$ is given by finding a state $\tau \in D$ that minimizes the relative entropy between $\rho$ and $\tau$. That is,

$$E_R(\rho) = \min_{\sigma} S(\rho||\sigma) = \min_{\sigma \in D} \text{Tr}(\rho \log \rho - \rho \log \sigma)$$

(2.2)

where $\sigma$ is a state in $D$. However, finding $\sigma$ to minimize $S(\rho||\sigma)$ is a difficult task, mainly due to the fact that characterizing the set of SEP is hard [20]. In practice, even for systems with dimension $d_A d_B > 6$, it is already hard to find whether a given state is separable or not [21].

$E_R(\rho)$ could be seen as a distance between the state $\rho$ and the set of SEP. Finding the distance means finding a point from the set which is the closest to the state. As shown in Fig. 1, for a state $\rho_A$ represented by the point $A$, the task is to find the point $A'$ (representing the state $\sigma_A$), to minimize

$$E_R(\rho_A) = \text{Tr}(\rho \log \rho_A - \rho \log \sigma_A').$$

(2.3)

Since the characterization of the set of SEP is know to be very difficult, so does the calculation of $E_R(\rho)$. It has been proposed to approximates the set of SEP by the set of states with positive partial transpose (denoted by PPT) [17], which is easier to characterize. However, it is well known that the set PPT is strictly larger than the set of SEP for $d_A d_B > 6$. Hence the method based on PPT hence gives an lower bound for $E_R(\rho)$, and does not given any information for bound entangled states.

In order to obtain upper bounds for $E_R(\rho)$, one would then need to approximate the set of SEP from the inside. We then propose to calculate $E_R(\rho)$ based on convex hull approximation as proposed in [19]. The algorithm goes
We use functions in CVXQUAD to calculate the relative entropy of entanglement [24]. The functions for generating Werner states and isotropic states are from QETLAB [25].

III. RESULTS

In this section, we apply our method to various situations of interest. We focus on bipartite systems of dimension $d_A d_B$. We take three steps: firstly we apply our method to calculate $E_R(\rho)$ for states whose relative entropy of entanglement is analytically known, and compare our results with both the analytical value and the value given by the PPT method. Then we take a step further to evaluate $E_R(\rho)$ for a set of example of bound entangle states, where the PPT method cannot give useful information for $E_R(\rho)$, and demonstrate that our bound likely give a good approximation for the real value of $E_R(\rho)$. Finally, we apply our method to randomly generated states for different values of $d_A d_B$, to show that the difference between the set of SEP and the set of PPT, for $d_A d_B > 6$.

A. States with analytically known $E_R$

To demonstrate the validity of our algorithm for calculating the upper bound of $E_R$, we first look at two kind of states whose $E_R$ are analytically known.

We start with the famous Werner states for $d \otimes d$ dimensional bipartite systems, which are states invariant under any unitary transform with the form $U \otimes U$ [26]. There are several ways for parametrizing these states. Here, we use the following form to write a Werner states as

$$\rho_W(\alpha) = \frac{1}{d^2 - d\alpha} (I_{d^2} - \alpha F),$$

where $d$ is the dimension, and $F = \sum_{ij} |ij\rangle\langle ji|$ (which is actually a swap operator).

Whether a Werner state is entangled is determined by the parameter $\alpha$, and can be given by the PPT criterion. That is, if a Werner state has positive partial transpose, then it is separable, otherwise it is entangled. Therefore, when calculating $E_R$ for Werner states, optimization over either the set of SEP or PPT should give the same result.

It is known that for $2 \otimes 2$ Werner states, the state is separable if $\alpha \leq 1/2$ and entangled if $\alpha > 1/2$. For $3 \otimes 3$ Werner states, the state is separable if $\alpha \leq 1/3$ and entangled if $\alpha > 1/3$ [26].

Due to the symmetry, $E_R$ for Werner states can be calculated analytically, which is given by [27]

$$E_R(\rho_W) = c_R(\text{tr}(\rho_W F)),$$
where $F = \sum_{ij} |ij\rangle\langle ij|$, and $e_{\mathcal{R}}$ is the function

$$
e_{\mathcal{R}}(f) = \log(2) - S\left(\frac{1+f}{2}, \frac{1-f}{2}\right), \quad (3.3)$$

with $S(p_1, p_2, \ldots, p_n) = -\sum_k p_k \log p_k$. In other words, for Werner states, the relative entropy of entanglement could be calculated by selecting $\sigma$ as the "boundary" Werner state. That is, for $2 \otimes 2$ Werner state, $\sigma = \rho_W(1/2)$ and for $3 \otimes 3$ Werner state, $\sigma = \rho_W(1/3)$.

We performed the calculation of $E_{\mathcal{R}}$ on $2 \otimes 2$ and $3 \otimes 3$ Werner states with three different methods: value from analytical formula, method based on PPT optimization, and our method based on CHA. The results are shown in Fig. 3.

As shown in Fig. 3, our approach using CHA as the approximation of $\mathcal{D}$ works perfectly for Werner states. The results of our approach, as well as the previous method based on PPT, agree well with the analytical results for different dimensions, see Fig. 3(a) and Fig. 3(b).

Notice that, which is shown in the middle small figure in Fig. 3(a), the results of our approach is slightly larger than that of PPT, to a scale of 0.01% of the actual analytical value. The reason is that our approach approximates the set $\mathcal{D}$ from inside and in fact calculates a upper bound. Therefore our results are always slightly larger than that is given by the PPT method.

We then further look at isotropic states, which is a family of $d \otimes d$ dimension bipartite quantum states that are invariant under any unitary transform with the form $U \otimes U^\dagger$ [28]. The parametrized form of isotropic states is given by

$$\rho_1(\alpha) = \frac{1 - \alpha}{d^2} I_d + \alpha |\psi_+\rangle \langle \psi_+|, \quad (3.4)$$

where $d$ is the dimension, and $|\psi_+\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |ii\rangle$, which is actually a standard maximally entangled state.

Similar to the case of Werner states, whether an isotropic state is entangled is determined by the parameter $\alpha$, and can also be given by the PPT criterion. Therefore, when calculating $E_{\mathcal{R}}$ for Werner states, optimization over either the set of SEP or PPT should give the same result.

It is known that for both $2 \times 2$ and $3 \times 3$ isotropic states, the state is separable if $\alpha \leq 1/3$ and entangled is $\alpha > 1/3$. With good symmetry, the result of relative entropy of entanglement of a certain isotropic state can be calculated analytically [29]. For an isotropic state $\rho_1$, let $\tilde{f} = \text{tr}(\rho_1 F)$ with $F = \sum_{ij} |ij\rangle\langle ij|$. Then $E_{\mathcal{R}}$ is given by

$$E_{\mathcal{R}}(\rho_1) = \log(2) - \left(1 - \frac{\tilde{f}}{d}\right) \log(d-1)$$

$$- S\left(\frac{\tilde{f}}{d}, 1 - \frac{\tilde{f}}{d}\right). \quad (3.5)$$

Similarly to Werner states, the calculation of relative entropy of entanglement of isotropic states could be carried out by choosing $\sigma$ as the boundary state, i.e. $\sigma = \rho(1/3)$.

We performed the calculation of the relative entropy of entanglements on $2 \otimes 2$ and $3 \otimes 3$ Werner states with different methods: value from analytical formula, method based on PPT optimization, and our method based on CHA. The results are shown in Fig. 4.

Similar to the results of Werner states, our approach using CHA as the approximation of $\mathcal{D}$ works well for isotropic states. The results of our approach, as well as SDP using PPT, agree well with the analytical results for different dimensions, as shown in Fig. 3(a) and Fig. 3(b).

**B. Example for bound entangled states**

We now apply our algorithm to find lower bound of $E_N$ for bound entangled state, which are entangled states with positive partial transpose. In this case, the method based on PPT will just give a value zero for a lower bound of $E_N$, which in fact fails to give any information of $E_N$. Our method based on CHA, instead, gives an upper bound for $E_N$, which in many cases can give results close to the true value of $E_N$.

We consider the following example, where a set of two-qutrits pure states $\{|v_1\rangle, \ldots, |v_5\rangle\}$ form the well known unextendible product basis [30]:

$$|v_1\rangle = (|00\rangle - |01\rangle)/\sqrt{2},$$

$$|v_2\rangle = (|21\rangle - |22\rangle)/\sqrt{2},$$

$$|v_3\rangle = (|02\rangle - |12\rangle)/\sqrt{2},$$

$$|v_4\rangle = (|10\rangle - |20\rangle)/\sqrt{2},$$

$$|v_5\rangle = (|0\rangle + |1\rangle + |2\rangle)\otimes 2/3. \quad (3.6)$$

It is known that

$$\rho_{\text{tiles}} = (I - \sum_{i=1}^5 |v_i\rangle\langle v_i|)/4 \quad (3.7)$$

is a bound entangled state. Therefore, the calculation of $E_N$ for $\rho_{\text{tiles}}$ based on the PPT method returns the value zero.

Consider the following set of states with parameter $\alpha$:

$$\rho_1(\alpha) = \alpha \rho_{\text{tiles}} + \frac{1 - \alpha}{9} I. \quad (3.8)$$

It is known that the critical point for whether $\rho_1(\alpha)$ is entangled or not is $\alpha \approx 0.8649$ [19].

We calculated $E_N$ for $\rho_1(\alpha)$ using based on CHA, and the results are shown in Fig. 5. In the middle small figure of Fig. 5, we see that the relative entropy entanglement goes from zero to non-zero value from around 0.86, which agree well with critical value $\alpha \approx 0.8649$. These results demonstrate the effective of the CHA approach for finding upper bounds of $E_N$ that is close to the true values.
C. Random States

We apply our algorithm to find upper bounds of $E_R$ for bipartite system of various dimensions of $d_A,d_B$, and compare with the lower bounds based on the PPT method.

We consider 4 cases, with dimensions $2 \otimes 2$, $2 \otimes 3$, $2 \otimes 4$, and $3 \otimes 3$. For each case, we randomly generated 50 entangled states using a similar method discussed in [19]. We then calculate the upper bound of $E_R$ based on the CHA method, and the lower bound of $E_R$ based on the PPT method. All the results are shown in Fig. 6.

Since for $d_A d_B \leq 6$, the set of SEP is the same as the set of PPT, the upper bound and lower bound should be very close to each other. This is indeed what we see for the case of $2 \otimes 2$ and $2 \otimes 3$, as shown in Fig. 6(a) and Fig. 6(b). For most cases, the two bound coincide to give the true value of $E_R$. For some states, the results of CHA is slightly larger than that of PPT. The results clearly meet the predictions of our theoretical analysis, demonstrating the effectiveness of our method.

For $d_A d_B > 6$, the set of SEP is strictly smaller than that of PPT. For random states, one would expect gap between the upper bounds given by CHA and the lower bounds given by PPT. This indeed what we see in the cases of $2 \otimes 4$ and $3 \otimes 3$, as shown in Fig. 6(c), Fig. 6(d), Fig. 6(e), and Fig. 6(f).

In the cases of $2 \otimes 4$ and $3 \otimes 3$, we see that for most states, the results of CHA is still very close to that of PPT. However, for some states, the results of CHA is significantly larger than that of PPT. And the gap is in fact larger in the case of $3 \otimes 3$ compared to the case of $2 \otimes 4$. In the cases of $3 \otimes 4$ and $4 \otimes 4$, for almost all states sampled, the upper bounds of $E_R$ calculated from CHA are larger than that of PPT. These observation agree with the previous observation on the volume of SEP compared to PPT [31]. With the values of upper bound of $E_R$, our results also provide new tools to study such vol-
FIG. 6: Results for random entangled states.

ume and deepen our understanding of the difference between SEP and PPT.

IV. DISCUSSION

In this work, we propose a new method for calculating upper bounds for relative entropy of entanglement, based on the CHA for the set of separable states. We apply our method to calculate composite system of various sizes, and compare to the previous known lower bounds, obtaining promising results. Since the CHA approach is a general idea to approximate convex set from inside, our method is naturally generalizable for obtaining upper bounds for any quantity of interest with optimization over convex set, especially in the case that extreme points of these sets are relatively easy to sample. We hope that our work add new understanding on the structure of separable states, provide further information on the difference between the set of separable states and PPT states in various dimensions, and shed light on the calculation of relevant quantities based on optimization over convex sets.

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[1] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Reviews of modern physics 81, 865 (2009).

[2] S. Lloyd, Physical Review A 55, 1613 (1997).
[3] E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, Science 292, 472 (2001).
[4] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Physical Review A 54, 3824 (1996).
[5] S. D. Huver, C. F. Wildfeuer, and J. P. Dowling, Physical Review A 78, 063828 (2008).
[6] B. Zeng, X. Chen, D.-L. Zhou, and X.-G. Wen, Quantum Information Meets Quantum Matter: From Quantum Entanglement to Topological Phases of Many-Body Systems (Springer, 2019).
[7] A. Almheiri, X. Dong, and D. Harlow, Journal of High Energy Physics 2015, 163 (2015).
[8] O. Gühne and G. Tóth, Physics Reports 474, 1 (2009).
[9] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight, Physical Review Letters 78, 2275 (1997).
[10] V. Vedral and M. B. Plenio, Physical Review A 57, 1619 (1998).
[11] V. Vedral, Reviews of Modern Physics 74, 197 (2002).
[12] M. Horodecki, P. Horodecki, and R. Horodecki, Physical Review Letters 84, 2014 (2000).
[13] E. M. Rains, IEEE Transactions on Information Theory 47, 2921 (2001).
[14] L. Henderson and V. Vedral, Physical review letters 84, 2263 (2000).
[15] M. W. Girard, G. Gour, and S. Friedland, Journal of Physics A: Mathematical and Theoretical 47, 505302 (2014).
[16] P. Horodecki, Physics Letters A 232, 333 (1997).
[17] H. Fawzi and O. Fawzi, Journal of Physics A: Mathematical and Theoretical 51, 154003 (2018). URL https://doi.org/10.1088%2F1751-8121%2Fa91e07.
[18] A. Miranowicz and A. Grudka, Journal of Optics B: Quantum and Semiclassical Optics 6, 542 (2004).
[19] S. Lu, S. Huang, K. Li, J. Li, J. Chen, D. Lu, Z. Ji, Y. Shen, D. Zhou, and B. Zeng, Phys. Rev. A 98, 012315 (2018). URL https://link.aps.org/doi/10.1103/PhysRevA.98.012315.
[20] L. Gurvits, in Proceedings of the thirty-fifth annual ACM symposium on Theory of computing (ACM, 2003), pp. 10–19.
[21] N. Johnston, Entanglement detection (2014).
[22] M. Grant and S. Boyd, CVX: Matlab software for disciplined convex programming. version 2.1, http://cvxr.com/cvx (2014).
[23] M. Grant and S. Boyd, in Recent Advances in Learning and Control, edited by V. Blondel, S. Boyd, and H. Kimura (Springer-Verlag Limited, 2008), Lecture Notes in Control and Information Sciences, pp. 95–110, http://stanford.edu/~boyd/graph_dcp.html.
[24] H. Fawzi, J. Saunderson, and P. A. Parrilo, Foundations of Computational Mathematics (2018), package cvxquad at https://github.com/hfawzi/cvxquad.
[25] N. Johnston, QETLAB: A MATLAB toolbox for quantum entanglement, version 0.9, http://qetlab.com (2016).
[26] R. F. Werner, Phys. Rev. A 40, 4277 (1989), URL https://link.aps.org/doi/10.1103/PhysRevA.40.4277.
[27] K. G. H. Vollbrecht and R. F. Werner, Physical Review A 64, 062307 (2001).
[28] M. Horodecki and P. Horodecki, Phys. Rev. A 59, 4206 (1999), URL https://link.aps.org/doi/10.1103/PhysRevA.59.4206.
[29] E. M. Rains, Phys. Rev. A 60, 179 (1999), URL https://link.aps.org/doi/10.1103/PhysRevA.60.179.
[30] C. H. Bennett, D. P. DiVincenzo, T. Mor, P. W. Shor, J. A. Smolin, and B. M. Terhal, Physical Review Letters 82, 5385 (1999).
[31] S. J. Szarek, I. Bengtsson, and K. Życzkowski, Journal of Physics A: Mathematical and General 39, L119 (2006).