Numerical results for geometric measure of coherence and geometric measure of entanglement based on semidefinite programs

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We present semidefinite programs for computing the geometric measure of coherence and the geometric measure of entanglement, respectively. For the geometric measure of coherence, the algorithm can be applied to any finite-dimensional mixed state. We test randomly generated single-qubit states, single-qutrit states, and a special kind of d-dimensional mixed states. For the geometric measure of entanglement, the algorithm is applied to all two-qubit and qubit-qutrit states, and some special kinds of higher dimensional mixed states. For other states, the algorithm can get a lower bound of the geometric measure of entanglement. Randomly generated two-qubit states, the isotropic states and the Werner states are tested. Furthermore, the maximum deviation between the analytical solution and the numerical solution is calculated.

I. INTRODUCTION

Coherence and entanglement are two basic concepts in quantum information theory, which are extensively applied to quantum information processing and quantum computational tasks [1]. Therefore, characterizing and quantifying coherence and entanglement become significant parts in quantum information theory [2]. Recent studies consider quantum coherence and entanglement as quantum resources, which can be applied to quantum-enhanced metrology, quantum key distribution and so on [3–9].

Quantum coherence is defined for a single system and is widely used in quantum optics in previous studies [10–17]. For any distance measure $D$ between quantum states $\rho$ and $\delta$, a general coherence measure is defined as $C_D(\rho) = \min_{\delta \in I} D(\rho, \delta)$, i.e., the minimum distance from $\rho$ to all incoherent states $\delta \in I$, where $I$ is the set of all incoherent states [18–22]. If and only if $\rho$ is an incoherent state, $C_D(\rho) = 0$. Then, some distance-based coherence quantifiers are proposed such as geometric coherence, relative entropy of coherence and $l_1$ norm of coherence. The geometric measure of coherence is defined in fidelity between the measured state and the nearest incoherent state [23]. The relative entropy of coherence is another distance-based coherence quantifier [18]. In addition, it is equal to the distillable coherence, so they have the similar expression [18–24]. Considering the coherence quantifiers based on the matrix norm, the $l_1$ norm of coherence was introduced and studied in Ref. [18]. Besides, other different coherence measures have been proposed [25–28].

Quantum entanglement is widely regarded as the essential feature of quantum mechanics. A class of entanglement measures are based on the fact that the closer a state is to the set $\mathcal{S}$ of separable states, the less entanglement it has [19–22]. According to the distance measure $D$ between quantum states $\rho$ and $\sigma$, it is defined as $E_D(\rho) = \min_{\sigma \in \mathcal{S}} D(\rho, \sigma)$, i.e., the measure is the minimum distance to all separable states [18–22]. One fundamental distance-based entanglement measure is the relative entropy of entanglement [22], which can be considered as a strong upper bound for entanglement of distillation [27]. Another one is the geometric measure of entanglement (GME) [30–31]. Furthermore, the expected value of entanglement witnesses can be used to estimate the GME [32]. Other different entanglement measures have been proposed for multipartite systems and mixed states [19–20].

Most quantum states have no corresponding analytical solution for the coherence and entanglement measures, so numerical algorithms must be applied. In some entanglement measures, several numerical algorithms have been used to solve related problems [33–36]. Moreover, computing many entanglement measures is NP hard for a general state [37–38], so some upper and lower bounds are proposed to describe entanglement [39–40] and coherence measures [47–51].

In Ref. [52], a semidefinite program (SDP) was proposed to calculate the fidelity between two states, so the geometric measures of coherence and entanglement can be calculated by optimizing the semidefinite program. The SDP is also applied to optimal measurements for distinguishing ensembles of states [52]. In this paper, we test some examples to study the feasibility of the optimization program about fidelity.

The paper is organized as follows. In section II we review the definition and properties of fidelity and introduce its semidefinite program. In section III we test our semidefinite program on the geometric measure of coherence of single-qubit states, single-qutrit states, and a special kind of d-dimensional mixed states. In section IV we introduce the states with positive partial transpose (PPT), and calculate the analytical and numerical solutions of two-qubit state of GME. Meanwhile, the maximum deviation between numerical and analytical solutions of different isotropic states and the Werner states are also calculated. A brief conclusion is proposed in Section V.

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II. A SEMIDEFINITE PROGRAM FOR COMPUTING FIDELITY

Here we sketch the fidelity and its semidefinite program applied in the following. The fidelity between states $\rho$ and $\chi$ is defined as

$$ F(\rho, \chi) \equiv \text{Tr} \sqrt{\rho^{\frac{1}{2}} \chi \rho^{\frac{1}{2}}}, \quad (1) $$

$$ \chi = \delta, \sigma. $$

For a pure state $|\psi\rangle$ and an arbitrary state $\chi$, it will see that

$$ F(|\psi\rangle, \chi) = \sqrt{\langle\psi|\chi|\psi\rangle}, \quad (2) $$

Here we consider a semidefinite program, whose optimal value equals the fidelity for given positive semidefinite operators $\rho, \chi$, i.e., considering the following optimization problem

maximize: \[ \frac{1}{2} \text{Tr}(X) + \frac{1}{2} \text{Tr}(X^\dagger), \]

subject to: \[ \begin{pmatrix} \rho & X \\ X^\dagger & \chi \end{pmatrix} \geq 0, \]

$$ X \in L(\mathbb{X}), \]

$$ \rho, \chi \in \text{Pos}(\mathbb{X}), $$

where $L$ is the collection of all linear mappings. In a complex Hilbert space, $\text{Pos}(\mathbb{X})$ is the set of positive semidefinite operators operating on $\mathbb{X}$. Then the maximum value of $\frac{1}{2} \text{Tr}(X) + \frac{1}{2} \text{Tr}(X^\dagger)$ is equal to $F(\rho, \chi)$. $X$ is a randomly generated complex matrix of the same order as $\chi$. The SDP can not only solve the problem effectively, but also prove the global optimality under weak conditions $[52]$. This implies that SDP optimization problems can be tackled with standard numerical packages. In this paper, the optimization of the SDP $[52]$ can be solved by using the Matlab parser YALMIP $[54]$ with the solvers, SEDUMI $[55]$ or SDPT3 $[56]$. There exist several SDP programs in quantum information theory. For example, SDP programs have been used in entanglement detection and quantification $[57]$ $[62]$, quantifying quantum resources $[63]$. Furthermore, the SDP $[52]$ has also been used for calculating the fidelity of quantum channels $[64]$. 

III. GEOMETRIC MEASURES OF COHERENCE

In a $d$-dimension Hilbert space $\mathcal{H}$ with its corresponding reference basis $\{|i\rangle\}_{i=0}^{d-1}$, a state is incoherent if and only if it is a diagonal density matrix under the reference basis $[53]$. All incoherent states can be represented as

$$ \delta = \sum_{i=0}^{d-1} p_i |i\rangle \langle i|, \quad (4) $$

Thus, the geometric measure of coherence is defined as $[23]$

$$ C_g(\rho) = 1 - \max_{\delta \in \mathbb{I}} F(\rho, \delta), \quad (5) $$

with the maximum being taken over all possible incoherent states $\delta \in \mathbb{I}$. For an arbitrary single-qubit state $\rho$, its analytical solutions of $C_g(\rho)$ has been derived $[23]$

$$ C_g(\rho) = \frac{1}{2} (1 - \sqrt{1 - 4 |\rho_{01}|^2}), \quad (6) $$

where $\rho_{01}$ is the off-diagonal element of $\rho$ in reference basis. To compare with this analytical solution, we randomly generate $10^5$ density matrices and calculate their $C_g(\rho)$ by analytical and numerical methods, respectively. The analytical results are calculated based on Eq. (6), and the numerical results are obtained by optimizing the semidefinite program $[65]$. The maximum deviation between the analytical and numerical results is $3.19 \times 10^{-9}$. For a pure state $|\psi\rangle = \sum_i \lambda_i |i\rangle$, its geometric measure of coherence is

$$ C_g(|\psi\rangle) = 1 - \max_i |\lambda_i|^2, \quad (7) $$

where $|\lambda_i|^2$ is the diagonal elements of $|\psi\rangle \langle\psi|$. However, the corresponding analytical solutions of $C_g(\rho)$ are difficult to calculate for general mixed states, so it is necessary to get some lower and upper bounds of $C_g(\rho)$. Here we employ the lower and upper bounds proposed in Ref. $[49]$ and compare them with our numerical results of the optimization program. For a general $d \times d$ density matrix $\rho$, its $C_g(\rho)$ satisfies $[49]$

$$ 1 - \frac{1}{d} - \frac{d-1}{d} \sqrt{1 - \frac{d}{d-1} (\text{Tr} \rho^2 - \sum_i \rho_{ii}^2)} \leq C_g(\rho) \leq \min \{1 - \max_i \rho_{ii}, 1 - \sum_i b_{ii}^2\}, \quad (8) $$

where $b_{ij}$ is from $\sqrt{\rho} = \sum_{ij} b_{ij} |i\rangle \langle j|$. Since there is no corresponding analytic solution for general single-qutrit mixed states, we randomly generate $10^5$ density matrices to draw their corresponding upper and lower bounds. In Fig. 1 there is a clear dividing line between two bounds indicating that the numerical results obtained by our algorithm conforms to the inequality (8), and points on the upper bound is closer to the dividing
line than points on the lower bound for many 3×3 density matrices.

Now we consider the following mixed state

$$\rho = p|\psi^+\rangle\langle\psi^+| + (1-p)\mathbb{I}/d, \quad (9)$$

with $|\psi^+\rangle = \frac{1}{\sqrt{d}}\sum_{i=0}^{d-1}|i\rangle$, $\mathbb{I}$ being the $d \times d$ identity matrix, and $0 \leq p \leq 1$. Since the mixed state $\rho$ is highly symmetric, it will remain unchanged when we exchange its basis order. It limits that the reference incoherent state in geometric measure of coherence must have the same diagonal elements, i.e., the closest incoherent state $\delta$ to the density matrix $\rho$ has to be

$$\delta = \sum_{i=0}^{d-1} \frac{1}{d} |i\rangle\langle i|. \quad (10)$$

Therefore, we can obtain an analytic solution of geometric measure of coherence for the mixed state $\rho$

$$C_g(\rho) = 1 - \frac{1}{d^2}[(d - 1)\sqrt{1 - p} + \sqrt{1 + (d - 1)p}]^2, \quad (11)$$

by using Eqs. (1), (5), (9) and (10), and it is equal to its corresponding upper bound which is the right hand side of the inequality (5). When $2 \leq d \leq 20$, we calculate their analytical and numerical results as well as maximum deviation between them. For $d = 3$ the corresponding graph is drawn and the rest have the similar phenomena like it. In Fig. 2 $C_g(\rho)$ and its upper bound coincide for $d = 3$, and the maximum deviation between them is $1.51 \times 10^{-9}$. In Fig. 3 the maximum deviation between the numerical and analytical results is about $10^{-9}$ orders of magnitude. Although the average time $t(s)$ of each operation increases exponentially, it is within an acceptable range in the low dimensional case.

IV. GEOMETRIC MEASURES OF ENTANGLEMENT

A separable bipartite pure state can be written in the following product form

$$|\psi^{AB}\rangle = |\psi^A\rangle \otimes |\psi^B\rangle. \quad (12)$$

For mixed states, if it can be represented as convex weights $p_i$ and product states $\rho_i^A \otimes \rho_i^B$ [66]

$$\rho^{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B, \quad (13)$$

then $\rho^{AB}$ is called separable. For a bipartite state, if there is no negative eigenvalues after the partial transposition of subsystem $A$, this bipartite state is called the

\* \* \*
PPT states \[ \rho_{AB} = \sum_{i,j,k,l} \rho_{i,j,k,l} |i⟩⟨j|_A \otimes |k⟩⟨l|_B, \] (14) is PPT, when its partial transposition with respect to the subsystem \( A \) satisfies
\[ \rho_{A|B}^{T_A} = \sum_{i,j,k,l} \rho_{i,j,k,l} |i⟩⟨j|_A \otimes |k⟩⟨l|_B \geq 0. \] (15)

The GME is defined as follows \[ 8 \]
\[ E_G(\rho) = 1 - [\max_{\sigma \in \mathcal{S}} F(\rho, \sigma)]^2, \] (16)
where \( \mathcal{S} \) is the set of all separable states. We replace the set \( \mathcal{P} \) of all PPT states, because \( \mathcal{S} \) cannot be easily expressed in the semidefinite programs, but \( \mathcal{P} \) can be expressed since for a given density matrix one can directly calculate its partial transpose \[ 32 \]. Thus, based on the fact that \( \mathcal{S} \) is a subset of \( \mathcal{P} \), one can obtain a lower bound of \( E_G(\rho) \), i.e.,
\[ E_G(\rho) \geq \tilde{E}_G(\rho), \] (17)
where the lower bound \( \tilde{E}_G(\rho) \) is defined by
\[ \tilde{E}_G(\rho) = 1 - [\max_{\sigma \in \mathcal{P}} F(\rho, \sigma)]^2. \] (18)
The equality in Eq. (17) holds for all two-qubit and qubit-qutrit states \[ 69 \], and some special kinds of higher dimensional mixed states.

For pure states, the GME is defined as \[ 2 \]
\[ E_G(\vert \psi \rangle \rangle) = 1 - \max_{\vert \psi \rangle \rangle \in \mathcal{S}} (\vert \langle \psi \vert \phi \rangle \rangle)^2, \] (19)
Moreover, it is defined via the convex roof construction for mixed states. If \( \rho \) is a two-qubit state, the corresponding expression of \( E_G(\rho) \) is \[ 2, 70, 71 \]
\[ E_G(\rho) = \frac{1}{2}(1 - \sqrt{1 - C(\rho)^2}). \] (20)
The \( C(\rho) \) is called concurrence that its expression is
\[ C(\rho) = \max \{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \] (21)
where \( \{\lambda_i\} \) are the square root of eigenvalues of \( \rho \) in descending order and \( \rho = (\sigma_0 \otimes \sigma_0)^a (\sigma_y \otimes \sigma_y)^b \). In order to compare the analytical result Eq. (20) and the numerical result for two-qubit states, we randomly generate \( 10^6 \) density matrices and calculate the analytical and numerical results respectively. The maximum difference between them is \( 1.57 \times 10^{-8} \).

Now we apply our semidefinite program to the isotropic states, where the forms of these states are \[ 2 \]
\[ \rho = \frac{1 - F}{d^2 - 1}(1 - |\Phi^+\rangle \langle \Phi^+|) + F|\Phi^+\rangle \langle \Phi^+|, \] (22)
with the maximally entangled state \( |\Phi^+\rangle = \frac{1}{\sqrt{d}} \sum_{i=0}^{d-1} |ii\rangle \) and \( 0 \leq F \leq 1 \). The analytical solutions for the GME of these isotropic states were given in Ref. \[ 2 \], and the states are separable if and only if \( F \leq \frac{1}{2} \) \[ 72 \]. For Eq. (22) when \( 2 \leq d \leq 5 \), we calculate that the maximum deviation between the numerical and analytical solution by our semidefinite program and the analytical solution given in \[ 2 \], respectively. The results are summarized in Table I, where \( \tilde{t}(s) \) denotes the average time of each operation. In the example tested above, the semidefinite program always obtain the same value as \( E_G(\rho) \) within the precision given in Table I.

Finally, we apply semidefinite program to the Werner states that can be expressed as a linear combination of two operators of the identity \( \mathbb{1} \) and the swap \( \hat{F} \equiv \sum_{i,j} |ij\rangle \langle ji| \), i.e., \( \rho = a \mathbb{1} + b \hat{F} \), where \( a \) and \( b \) are both real coefficients and are limited by \( \text{Tr} \rho = 1 \). When one of the parameters is considered, the states can be expressed as
\[ \rho = \frac{d^2 - f d}{d^4 - d^2} \mathbb{1} \otimes \mathbb{1} + \frac{f d^2 - d}{d^4 - d^2} \hat{F}, \] (23)
with \( f \equiv \text{Tr}(\rho \hat{F}) \). The corresponding analytic solution for the Werner states \[ 23 \] is \[ 2 \]
\[ E_G(\rho) = \frac{1}{2}(1 - \sqrt{1 - f^2}), \] (24)
where \( f \leq 0 \) and 0 otherwise. For \( 2 \leq d \leq 5 \), we apply our semidefinite program to states \[ 23 \], so the maximum deviation between the numerical solution and the analytical solution is calculated, respectively. The results are summarized in Table II, where \( \tilde{t}(s) \) is the average time of each operation.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\( d \) & 2 & 3 & 4 & 5 \\
\hline
\( \Delta E_G(\rho) \) & \( 1.03 \times 10^{-9} \) & \( 2.02 \times 10^{-9} \) & \( 3.21 \times 10^{-9} \) & \( 5.05 \times 10^{-9} \) \\
\hline
\( \tilde{t}(s) \) & 0.29 & 0.49 & 2.23 & 27.35 \\
\hline
\end{tabular}
\caption{The maximum deviation between the numerical solution and the analytical solution with \( \Delta E_G(\rho) = E_G(\rho) - \tilde{E}_G(\rho) \), and the average time \( \tilde{t}(s) \) of each operation for the isotropic states \[ 22 \].}
\end{table}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
\( d \) & 2 & 3 & 4 & 5 \\
\hline
\( \Delta E_G(\rho) \) & \( 5.00 \times 10^{-10} \) & \( 2.26 \times 10^{-9} \) & \( 3.17 \times 10^{-9} \) & \( 5.57 \times 10^{-9} \) \\
\hline
\( \tilde{t}(s) \) & 0.32 & 0.46 & 1.47 & 14.83 \\
\hline
\end{tabular}
\caption{The maximum deviation between the numerical solution and the analytical solution with \( \Delta E_G(\rho) = E_G(\rho) - \tilde{E}_G(\rho) \), and the average time \( \tilde{t}(s) \) of each operation for the Werner states \[ 23 \].}
\end{table}
V. CONCLUSIONS

In this paper, we introduced an algorithm to compute the geometric measures of coherence and the entanglement. In coherence measures, the deviation between the numerical solution and the analytical solution was an order of magnitude of $10^{-9}$ for single-qubit states. And we obtained its analytical solution is $C_g(\rho) = 1 - \frac{1}{d}((d-1)^{3/2} + 1 + (d-1)^{3/2})^2$ for the special state $\rho = p|\psi^+\rangle\langle\psi^+| + (1-p)\frac{1}{d}I$. For any 3-dimensional density matrix, we have drawn a boundary diagram with an apparently clear boundary line. In entanglement measures, we used PPT states to replace the set of separable states and calculated two-qubit states, the isotropic states and the Werner states by using fidelity and its semidefinite program, and then concluded that their maximum deviation is almost on the order of magnitude of $10^{-9}$. In short, whether in coherent or entanglement measure, the semidefinite program of this paper can always calculate the same answer as the analytical solution within the given precision range in this paper.

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Supplemental Material

Here we provide some detailed calculations of the single-qubit states, randomly generate 3-dimensional density matrices, and a special kind of $d$-dimensional density matrices for coherence measures. The corresponding MATLAB code for the semidefinite program of geometric measure of coherence is

```matlab
function [C, D]=coherence(rho)

d=length(rho);

delt=sdpvar(d,d, 'diagonal', 'real');

X=sdpvar(d,d, 'full', 'complex');

constr=[[rho X; ctranspose(X) delt]≥0, delt≥0, trace(delt)==1];

result=solvesdp(constr, -trace(X)-trace(ctranspose(X)), sdpsettings('verbose', 1));

%check for errors
if (result. problem ≠ 0 )
    disp(result. info);
end

%return the maximum fidelity
F=double((trace(X)+trace(ctranspose(X)))/2);

D=double(delt);

C=1-Fˆ2;
end
```

We have used the parser YALMIP [1] with the solvers, SEDUMI [2] or SDPT3 [3].

We also provide some detailed calculations of the two-qubit states, the isotropic states and the Werner states for entanglement measures. The corresponding MATLAB code for the semidefinite program of geometric measure of entanglement is

```matlab
function [E, E2]=GME(rho)

%d(i) is the dimension of the matrix
    d1=2;
    d2=2;

    sigma=sdpvar(d1*d2, d1*d2, 'hermitian', 'complex');

    X=sdpvar(d1*d2, d1*d2, 'full', 'complex');

%performing partial transpose for sigma and the pt subroutine comes from pptmixer.
    constr=[[rho X; ctranspose(X) sigma]≥0, sigma≥0, pt(sigma, [1,0], [d1, d2])≥0, trace(sigma)==1];

    result=solvesdp(constr, -trace(X)-trace(ctranspose(X)), sdpsettings('verbose', 1));

%check for errors
if (result. problem ≠ 0 )
    disp(result. info);
end

%return the maximum fidelity
    F=double((trace(X)+trace(ctranspose(X)))/2);

    D=double(sigma);

    E=1-Fˆ2;
end
```
We have used the pt subroutine from the program PPTmixer, where the PPTmixer was presented in [4] (or [5]).

[1] https://yalmip.github.io
[2] http://sedumi.ie.lehigh.edu
[3] http://www.math.nus.edu.sg/~mattohkc/sdpt3.html
[4] B. Jungnitsch, T. Moroder and O. Gühne, Phys. Rev. Lett. 106, 190502 (2011).
[5] See the program PPTmixer, (available at www.mathworks.com/matlabcentral/fileexchange/30968).