



# Two-qubit trace-norm geometric discord: the complete solution

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## Abstract

We present the complete solution of the problem of determination of trace-norm geometric discord for arbitrary two-qubit state. Final answer is achieved due to effective reduction of the problem to the study of critical points of certain mapping depending on projectors. Our results are illustrated on various, also new, families of two-qubit states and compared to already known special solutions.

**Keywords** Qubits · Quantum correlations · Geometric quantum discord · Trace norm

## 1 Introduction

It is a common belief that question of the explicit quantitative characterization of correlations for a two-qubit systems can always be answered, but actually in many cases we land on a uncharted territory, where the explicit answer is not known [1–3]. One of these situations is the strict solution of the question of trace-norm quantum geometric discord  $D_1$  for an arbitrary state of the two-qubit system. The two-qubit system is the simplest non-trivial compound system which we have at our disposal to study quantum correlations and all relevant tools invented to measure them [1]. The geometric quantum discord measured by means of the distance induced by the trace norm seems to be one of the solid candidates. Contrary to the geometric discord defined by means of the Hilbert–Schmidt distance, it is well defined and satisfies requirements of the bona fide measure of quantum correlations. As it is well known, the Hilbert–Schmidt distance yields to an anomalous behavior related to it geometric

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discord  $D_2$ , but it has an attractive property that it can be calculated relatively easy. The procedure for calculating geometric discord involves the minimization which for generic states for the trace distance is rather challenging. As we have shown for qutrits and higher-dimensional bipartite systems it can be hardly operationally/analytically performed, except for selected families of states [4].

In the present work we show how explicitly the  $D_1$  can be determined and we reveal the geometry of the problem of minimization, which in turn deepens the understanding of the intrinsic geometry of the two-qubit quantum state space. For the Hilbert–Schmidt distance quantum discord  $D_2$  such a question has been answered in a compact form by Dakić et al. [5], namely the explicit formula for the  $D_2$  has been obtained. The ease of computation does not heal the non-physical behavior of the  $D_2$  under the local evolution of the system [6] and its non-contractibility under completely positive trace preserving mappings.

The trace-norm measurement-induced geometric discord is well-defined correlation measure. For two qubits it is also equal to the standard geometric discord defined as the distance from a given state to the set of classical-quantum states [7,8] and it is more convenient to use quantity based on the disturbance induced by measurement. Such quantity will be simply called geometric quantum discord. However, its calculation is still rather challenging, and by now no explicit answer for arbitrary two-qubit state has been known. According to our best knowledge supported by the recent review on the quantum correlations and geometric quantum discord [3], prior to the present work only few answers were found for selected families of states:

- (a) for the Bell diagonal states (or states with maximally mixed marginals) [9],
- (b) for the X-shaped states [10],
- (c) for the states with the correlation matrix having only one nonzero singular value and arbitrary Bell vectors of the marginals—such class contains, in particular, so-called quantum-classical states [10].

The objective of this study is to provide the complete solution of the problem of giving the explicit value of geometric quantum discord  $D_1(\rho)$  for arbitrary two-qubit state  $\rho$ . We find the answer to the minimization problem which has nice geometric meaning. As an illustration, we analyze previously known partial solutions for above-mentioned families of states and indicate mechanism making that these solutions were so much simpler.

The paper is organized as follows: In Sect. 2, we briefly review basic notions and fix the relevant notation. Then, in Sect. 3, we prove the theorem giving characterization of the central formula for the trace norm of the disturbance of the system by a local projective measurements. To guide the reader gently to the full solution, in Sect. 4, we compute the  $D_1(\rho)$  for the relatively large family of states for which the minimization procedure is not necessary at all or is straightforward. Section 5 is central for the final result; there we study the critical points of the trace-norm disturbance mapping and obtain that there are two possibilities: singular critical points and smooth critical points. As a preliminary application, we apply new results to the states with maximally mixed marginals. In Sect. 6 we prove the main result: the determination of the trace-norm geometric discord in general case. Finally, Sect. 7 will allow reader to make contact with known solutions and go beyond the family of the X-shaped states. We finish the

paper with some conclusions and comments on the main findings and obstructions to their extensions to higher-dimensional systems.

## 2 Preliminary notions

In the description of two-qubit systems we follow general formulation of  $d$ -level quantum systems introduced in [4], specified to the case  $d = 2$ .

### 2.1 Two qubits

Qubit is a two-level quantum system. The corresponding Hilbert space equals to  $\mathbb{C}^2$ , and the observables are given by Hermitian elements of full matrix algebra  $\mathbb{M}_2(\mathbb{C})$ . As a basis in  $\mathbb{M}_2(\mathbb{C})$ , we use standard Pauli matrices  $\sigma_1, \sigma_2, \sigma_3$  and the identity matrix  $\mathbb{1}_2$ . In the following we will use the notation

$$\langle n, \sigma \rangle = n_1\sigma_1 + n_2\sigma_2 + n_3\sigma_3, \quad \sigma = (\sigma_1, \sigma_2, \sigma_3), \quad n = (n_1, n_2, n_3)$$

Then, from the properties of Pauli matrices it follows that

$$\langle n, \sigma \rangle \langle m, \sigma \rangle = \langle n, m \rangle \mathbb{1}_2 + i \langle n \times m, \sigma \rangle \tag{2.1}$$

The set  $\mathcal{E}_2$  of all states of two-level system can be parametrized as follows:

$$\rho = \frac{1}{2} (\mathbb{1}_2 + \langle n, \sigma \rangle), \quad n \in \mathbb{R}^3 \tag{2.2}$$

where  $\|n\| \leq 1$ . So  $\mathcal{E}_2$  is given by the unit ball in  $\mathbb{R}^3$  and the pure states correspond to the unit sphere  $\|n\| = 1$ .

Consider now two qubits  $\mathcal{A}$  and  $\mathcal{B}$ . It is convenient to parametrize the set of states of composite system as follows:

$$\rho = \frac{1}{4} \left( \mathbb{1}_2 \otimes \mathbb{1}_2 + \langle x, \sigma \rangle \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \langle y, \sigma \rangle + \sum_{j,k=1}^3 K_{jk} \sigma_j \otimes \sigma_k \right) \tag{2.3}$$

where  $x, y \in \mathbb{R}^3$  and  $K = (K_{jk})$  is the correlation matrix. Notice that

$$x_j = \text{tr} (\rho \sigma_j \otimes \mathbb{1}_2), \quad y_j = \text{tr} (\rho \mathbb{1}_2 \otimes \sigma_j), \quad K_{jk} = \text{tr} (\rho \sigma_j \otimes \sigma_k)$$

The parametrization (2.3) is chosen in such a way that the marginals  $\text{tr}_{\mathcal{A}}\rho$  and  $\text{tr}_{\mathcal{B}}\rho$  are given by the vectors  $x$  and  $y$  as in (2.2).

Let us discuss now the adjoint representation of the group  $SU(2)$ . Let  $\hat{U} \in SU(2)$  and define  $3 \times 3$  matrix  $U$  by

$$\langle Um, \sigma \rangle = \hat{U} \langle m, \sigma \rangle \hat{U}^*$$

The matrix  $U$  is real and orthogonal. In this way to each  $\hat{U} \in \text{SU}(2)$  there corresponds  $U \in \text{SO}(3)$ . In contrast to general case, when  $d = 2$  such obtained group is exactly equal to the group  $\text{SO}(3)$ . Consider now the local transformations of the state of two qubits

$$\rho \rightarrow \hat{U}^* \otimes \hat{V}^* \rho \hat{U} \otimes \hat{V}, \quad \hat{U}, \hat{V} \in \text{SU}(2) \tag{2.4}$$

The corresponding vectors  $x, y$  and the correlation matrix  $K$  transform as follows:

$$x \rightarrow x' = Ux, \quad y \rightarrow y' = Vy, \quad K \rightarrow K' = UKV^T \tag{2.5}$$

where  $U, V$  are the adjoint representations of  $\hat{U}, \hat{V}$ , respectively. Since in the case of qubits we can use the full group of orthogonal transformations to diagonalize correlation matrix, any two-qubit state is locally equivalent to the state with diagonal  $K$ .

### 2.2 Trace-norm geometric discord

Let  $\rho$  be a state of bipartite system  $\mathcal{AB}$ . When we perform local measurement on the subsystem  $\mathcal{A}$ , the state  $\rho$  may be disturbed due to such measurement. The trace-norm (one-sided) measurement-induced geometric discord is defined as the minimal disturbance induced by projective measurement  $\mathbb{P}_{\mathcal{A}}$  on subsystem  $\mathcal{A}$ , computed using the trace distance in the set of states. It can be compared with the standard geometric discord equal to the distance from a given state to the set of classical-quantum states [5]. At it was already stated in Introduction, in the case of qubits these two notions coincide, and it is more convenient to use the quantity based on the disturbance induced by the measurement which will be simply called trace-norm geometric discord. The formal definition is as follows [9]:

$$D_1(\rho) = \min_{\mathbb{P}_{\mathcal{A}}} \|\rho - \mathbb{P}_{\mathcal{A}}(\rho)\|_1 \tag{2.6}$$

where  $\|A\|_1 = \text{tr} |A|$ .

In the case of qubits, the local projective measurement  $\mathbb{P}_{\mathcal{A}}$  is given by the one-dimensional projectors  $P_1, P_2$  on  $\mathbb{C}^2$ , such that

$$P_1 + P_2 = \mathbb{1}_2, \quad P_j P_k = \delta_{jk} P_k$$

and  $\mathbb{P}_{\mathcal{A}} = \mathbb{P} \otimes \text{id}$ , where

$$\mathbb{P}(A) = P_1 A P_1 + P_2 A P_2 \tag{2.7}$$

One-dimensional projectors  $P_k$  can be always chosen as

$$P_k = u P_k^0 u^* \quad \text{for some } u \in \text{SU}(2)$$

where

$$P_1^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P_2^0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Define now a real orthogonal projector  $\mathcal{P}$  on  $\mathbb{R}^3$

$$\langle \mathcal{P}m, \sigma \rangle = \mathbb{P}(\langle m, \sigma \rangle), \quad m \in \mathbb{R}^3 \quad (2.8)$$

If  $\mathcal{P}_0$  denotes such projector given by (2.7), where we take  $P_1^0$  and  $P_2^0$ , then

$$\mathcal{P}_0 = \text{diag}(0, 0, 1)$$

and

$$\mathcal{P} = V\mathcal{P}_0V^T, \quad V \in \text{SO}(3) \quad (2.9)$$

Define also orthogonal complements to  $\mathcal{P}_0$  and  $\mathcal{P}$

$$\mathcal{M}_0 = \mathbb{1}_3 - \mathcal{P}_0, \quad \mathcal{M} = \mathbb{1}_3 - \mathcal{P} \quad (2.10)$$

Obviously  $\mathcal{M}_0 = \text{diag}(1, 1, 0)$ ,

$$\mathcal{M} = V\mathcal{M}_0V^T, \quad V \in \text{SO}(3)$$

and

$$\dim \text{Ran } \mathcal{M}_0 = \dim \text{Ran } \mathcal{M} = 2$$

Notice that in this case the projectors  $\mathcal{M}$  run over the whole set of projectors with dimension 2.

Now we compute the disturbance of the state (2.3) caused by measurement  $\mathbb{P}_{\mathcal{A}}$ . We have

$$\begin{aligned} S(\mathcal{M}) &= \rho - \mathbb{P}_{\mathcal{A}}(\rho) \\ &= \frac{1}{4} \left( \langle \mathcal{M}x, \sigma \rangle \otimes \mathbb{1}_2 + \sum_{k=1}^3 \langle \mathcal{M}Ke_k, \sigma \rangle \otimes \langle e_k, \sigma \rangle \right) \end{aligned} \quad (2.11)$$

where  $e_k$ ,  $k = 1, 2, 3$  are the vector of the canonical basis of  $\mathbb{R}^3$ . So

$$D_1(\rho) = \min_{\mathcal{M}} \text{tr} |S(\mathcal{M})| = \min_{\mathcal{M}} \text{tr} \sqrt{Q(\mathcal{M})} \quad (2.12)$$

where  $Q(\mathcal{M}) = S(\mathcal{M})S(\mathcal{M})^*$  and the minimum is taken over all projectors  $\mathcal{M}$  on two-dimensional subspaces of  $\mathbb{R}^3$ .

**Remark 2.1** Notice that the quantity  $D_1(\rho)$  does not depend on the choice of the state within the class of locally equivalent states. In other words

$$\min_{\mathcal{M}} \text{tr} \sqrt{Q(\mathcal{M})} = \min_{\mathcal{M}} \text{tr} \sqrt{Q'(\mathcal{M})}$$

where  $Q'$  is obtained from  $Q$  by taking vector  $x' = Ux$  and matrix  $K' = UKV^T$  instead of  $x$  and  $K$ .

### 3 Trace norm of disturbance $S(\mathcal{M})$

In this section we find the elegant formula for the trace norm of the disturbance  $S(\mathcal{M})$  (see [10] for the other version of such formula).

**Theorem 3.1** *The trace norm of the disturbance  $S(\mathcal{M})$  of the state (2.3) is given by the formula*

$$\|S(\mathcal{M})\|_1 = \frac{1}{\sqrt{2}} \sqrt{\|\mathcal{M}x\|^2 + \text{tr}(\mathcal{M}K K^T) + \sqrt{[\|\mathcal{M}x\|^2 + \text{tr}(\mathcal{M}K K^T)]^2 - 4[\|K^T \mathcal{M}x\|^2 + \text{tr}(E^T E - \mathcal{M}E^T E)]}} \tag{3.1}$$

where  $\|\cdot\|$  denotes the Euclidean norm in  $\mathbb{R}^3$  and  $E = \text{adj } K$  is the adjunct matrix of the correlation matrix  $K$  (i.e., the transpose of its cofactor matrix).

**Proof** We start the proof of this theorem with the formula for  $Q(\mathcal{M}) = S(\mathcal{M})S(\mathcal{M})^*$ . By a direct computation we obtain

$$Q(\mathcal{M}) = \frac{1}{16} \left( (\text{tr}(\mathcal{M}K K^T) + \langle \mathcal{M}x, x \rangle) \mathbb{1}_2 \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes 2 \langle K^T \mathcal{M}x, \sigma \rangle + \sum_{j,k} \text{tr}(K^T \mathcal{M} F_j \mathcal{M} K F_k) \sigma_j \otimes \sigma_k \right) \tag{3.2}$$

where  $F_k$  are the generators of  $\text{SO}(3)$ , given by

$$(F_j)_{kl} = -\varepsilon_{jkl}, \quad j, k, l = 1, 2, 3$$

which satisfy covariance relations

$$U^T F_j U = \sum_k U_{jk} F_k$$

To further simplify (3.2) consider locally equivalent state for which the correlation matrix is diagonal. So, for a proper transformations  $U_0, V_0 \in \text{SO}(3)$ , we have

$$x_0 = U_0 x \quad \text{and} \quad I_0 = U_0 K V_0^T \tag{3.3}$$

and  $I_0$  is diagonal

$$I_0 = \text{diag}(i_1, i_2, i_3)$$

Let  $E_0 = \text{adj}(I_0)$  be the adjunct matrix of  $I_0$ . Then

$$E_0 = \text{diag}(\varepsilon_1, \varepsilon_2, \varepsilon_3)$$

where  $\varepsilon_1 = i_2 i_3, \varepsilon_2 = i_1 i_3, \varepsilon_3 = i_1 i_2$ . First, we show the identity

$$\text{tr}(I_0 \mathcal{M} F_j \mathcal{M} I_0 F_k) = -2\varepsilon_k V_{j3} V_{k3} \tag{3.4}$$

where  $\mathcal{M} = V\mathcal{M}_0V^T$ ,  $V \in \text{SO}(3)$ . The formula (3.4) follows since

$$I_0F_jI_0 = \varepsilon_jF_j, \quad j = 1, 2, 3$$

and

$$M_0F_kM_0 = 0, \quad k = 1, 2 \quad \text{whereas} \quad M_0F_3M_0 = F_3$$

For any orthogonal transformation  $V$  define the mapping  $\tau_V : \mathbb{M}_2(\mathbb{C}) \rightarrow \mathbb{M}_2(\mathbb{C})$  as follows:

$$\tau_V(a\mathbb{1}_2 + \langle m, \sigma \rangle) = a\mathbb{1}_2 + \langle Vm, \sigma \rangle$$

Now using the identity (3.4) we can transform the formula (3.2) to obtain

$$Q(\mathcal{M}) = \frac{1}{16} \left( (\text{tr}(MI_0^2) + \langle \mathcal{M}x_0, x_0 \rangle) \mathbb{1}_2 \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes 2 \langle I_0\mathcal{M}x_0, \sigma \rangle - 2\tau_V(\sigma_3) \otimes \tau_{E_0V}(\sigma_3) \right) \quad (3.5)$$

Observe that

$$\tau_V(\sigma_3) = \langle Ve_3, \sigma \rangle = \langle v, \sigma \rangle$$

where vector  $v$  is given by the third column of the matrix  $V$ . Similarly

$$\tau_{E_0V}(\sigma_3) = \langle E_0v, \sigma \rangle$$

Let us now introduce the matrix

$$R_0(\mathcal{M}) = \mathbb{1}_2 \otimes \langle I_0\mathcal{M}x_0, \sigma \rangle - \sigma_3 \otimes \langle E_0v, \sigma \rangle \quad (3.6)$$

This matrix has a block diagonal form with blocks

$$\langle I_0\mathcal{M}x_0 - E_0v, \sigma \rangle \quad \text{and} \quad \langle I_0\mathcal{M}x_0 + E_0v, \sigma \rangle \quad (3.7)$$

Put

$$R(\mathcal{M}) = (\tau_V \otimes \text{id}) R_0(\mathcal{M})$$

then

$$Q(\mathcal{M}) = \frac{1}{16} \left( (\text{tr}(\mathcal{M}I_0^2) + \langle \mathcal{M}x_0, x_0 \rangle) \mathbb{1}_2 \otimes \mathbb{1}_2 + 2 R(\mathcal{M}) \right)$$

The spectral analysis of  $R_0(\mathcal{M})$  is easy since characteristic polynomials for the blocks are given by

$$w_{\pm}(\lambda) = \det ((I_0\mathcal{M}x_0 \pm E_0v, \sigma) - \lambda \mathbb{1}_2) = \lambda^2 - \|I_0\mathcal{M}x_0 \pm E_0v\|^2$$

where the  $+(-)$  sign corresponds to the lower (upper) block. One can also check that the vectors  $I_0\mathcal{M}x_0$  and  $E_0v$  are orthogonal, so

$$w_+(\lambda) = w_-(\lambda) = \lambda^2 - \|I_0\mathcal{M}x_0\|^2 - \|E_0v\|^2$$

and the eigenvalues of  $R_0(\mathcal{M})$  are doubly degenerate

$$\lambda_{\pm}^{(+)} = \lambda_{\pm}^{(-)} = \pm \sqrt{\|I_0\mathcal{M}x_0\|^2 + \|E_0v\|^2}$$

Thus, we get

$$\text{tr} \sqrt{Q(\mathcal{M})} = \frac{1}{2} (\omega_+ + \omega_-) \tag{3.8}$$

where

$$\omega_{\pm} = \sqrt{\|\mathcal{M}x_0\|^2 + \text{tr}(I_0^2\mathcal{M}) \pm 2\sqrt{\|I_0\mathcal{M}x_0\|^2 + \|E_0v\|^2}}$$

The formula (3.8) can be further simplified, and we arrive at

$$\text{tr} \sqrt{Q(\mathcal{M})} = \frac{1}{\sqrt{2}} \sqrt{\|\mathcal{M}x_0\|^2 + \text{tr}(I_0^2\mathcal{M}) + \sqrt{[\|\mathcal{M}x_0\|^2 + \text{tr}(I_0^2\mathcal{M})]^2 - 4[\|I_0\mathcal{M}x_0\|^2 + \|E_0v\|^2]}} \tag{3.9}$$

Now applying the inverse to the transformation (3.3), we finally obtain the formula (3.1). □

### 4 Solving the minimization problem in the simple case

To compute the geometric discord of a given state, we have to find minimum of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ . In general it is a hard problem and its general solution will be described in the next sections. Now, let us consider a class of two-qubit states for which the solution of this problem is straightforward. This class (denoted by  $\mathcal{E}_0$ ) contains the states (2.3) with arbitrary Bloch vectors  $x, y$  and the correlation matrix of the form

$$K = t V_0$$

where  $V_0$  is some orthogonal matrix and  $t$  is a real parameter. From general properties of the two-qubit states, it follows that  $t$  belongs to the interval  $|t| \leq 1$ , but the actual value of  $t$  depends on the choice of the matrix  $V_0$  and vectors  $x, y$ . To apply the formula (3.1), notice that



$$K K^T = t^2 V_0 V_0^T = t^2 \mathbb{1}_3$$

and

$$(\text{adj } K)^T \text{adj } K = \text{adj}(K K^T) = \text{adj}(t^2 V_0 V) = t^4 \text{adj } \mathbb{1}_3 = t^4 \mathbb{1}_3$$

so

$$\text{tr}(\mathcal{M} K K^T) = t^2 \text{tr } \mathcal{M} = 2t^2, \quad \text{tr}(\mathcal{M}(\text{adj } K)^T \text{adj } K) = t^4 \text{tr } \mathcal{M} = 2t^4$$

moreover

$$\text{tr}((\text{adj } K)^T \text{adj } K) = t^4 \text{tr } \mathbb{1}_3 = 3t^4, \quad \|K^T \mathcal{M} x\| = |t| \|\mathcal{M} x\|$$

Now the formula (3.1) gives

$$\begin{aligned} \|S(\mathcal{M})\|_1^2 &= \frac{1}{2} \left( \|\mathcal{M} x\|^2 + 2t^2 + \sqrt{[\|\mathcal{M} x\|^2 + 2t^2]^2 - 4t^4 - 4t^2 \|\mathcal{M} x\|^2} \right) \\ &= \frac{1}{2} \left( \|\mathcal{M} x\|^2 + 2t^2 + \sqrt{\|\mathcal{M} x\|^4} \right) \\ &= t^2 + \|\mathcal{M} x\|^2 \end{aligned}$$

so

$$\|S(\mathcal{M})\|_1^2 \geq t^2$$

and minimal value is achieved for such  $\mathcal{M}$  which projects on  $x^\perp$  in  $\mathbb{R}^3$ . Thus, we have

**Theorem 4.1** For every state  $\rho \in \mathcal{E}_0$ , geometric discord is given by

$$D_1(\rho) = |t|$$

Characterization of the class  $\mathcal{E}_0$  is not an easy task. Partial information can be obtained considering locally equivalent states with diagonal correlation matrix. Therefore, let us consider the correlation matrix  $K$  of the form

$$K = t I$$

where  $I = \text{diag}(i_1, i_2, i_3)$ ,  $i_1, i_2, i_3 = \pm 1$ . In the following we restrict our analysis to  $I_1 = \mathbb{1}_3$  and  $I_2 = \text{diag}(1, -1, 1)$ . In the first case we obtain the family of states

$$\rho_1 = \frac{1}{4} \begin{pmatrix} 1+a+t & \bar{w} & \bar{z} & 0 \\ w & 1+b-t & 2t & \bar{z} \\ z & 2t & 1-b-t & \bar{w} \\ 0 & z & w & 1-a+t \end{pmatrix} \quad (4.1)$$

where  $a, b \in \mathbb{R}$ ,  $w, z \in \mathbb{C}$ . Similarly, in the second case, we have

$$\rho_2 = \frac{1}{4} \begin{pmatrix} 1+a+t & \bar{w} & \bar{z} & 2t \\ w & 1+b-t & 0 & \bar{z} \\ z & 0 & 1-b-t & \bar{w} \\ 2t & z & w & 1-a+t \end{pmatrix} \quad (4.2)$$

Notice that the relation between parameters  $a, b, w, z$  and Bloch vectors  $x, y$  is as follows:

$$x_1 = \operatorname{Re} z, \quad x_2 = \operatorname{Im} z, \quad x_3 = \frac{1}{2}(a+b)$$

and

$$y_1 = \operatorname{Re} w, \quad y_2 = \operatorname{Im} w, \quad y_3 = \frac{1}{2}(a-b)$$

To obtain more specific information we must restrict the number of parameters. The simplest is the case when Bloch vectors equal to zero vector. Then, (4.1) contains the one-parameter family of Werner states

$$\rho_W = \frac{1}{4} \begin{pmatrix} 1+t & 0 & 0 & 0 \\ 0 & 1-t & 2t & 0 \\ 0 & 2t & 1-t & 0 \\ 0 & 0 & 0 & 1+t \end{pmatrix}, \quad -1 \leq t \leq \frac{1}{3}$$

On the other hand, (4.2) contains the family of isotropic states

$$\rho_{\text{iso}} = \frac{1}{4} \begin{pmatrix} 1+t & 0 & 0 & 2t \\ 0 & 1-t & 0 & 0 \\ 0 & 0 & 1-t & 0 \\ 2t & 0 & 0 & 1+t \end{pmatrix}, \quad -\frac{1}{3} \leq t \leq 1$$

Isotropic states can be obtained as a mixture of maximally mixed state  $\rho_\infty = \frac{1}{4}\mathbb{1}_4$  and maximally entangled state  $\Psi_+$  given by

$$\Psi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

i.e.,

$$\rho_{\text{iso}} = (1-t)\rho_\infty + t|\Psi_+\rangle\langle\Psi_+|$$

On the other hand, the Werner states  $\tilde{\rho}_W$  with reversed parametrization ( $t \rightarrow -t$ ) can be obtained as the mixture of  $\rho_\infty$  and the state  $\Phi_-$ , where

$$\Phi_- = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

So both states are locally equivalent.

More interesting is the case of states with non-trivial Bloch vectors. For simplicity we consider the vectors of the form

$$x = y = (0, 0, \alpha), \quad |\alpha| \leq 1$$

In this case the properties of the states (4.1) and (4.2) differ significantly. In particular,  $\rho_1$  is positive definite when

$$|\alpha| \leq \frac{2}{3} \quad \text{and} \quad 2|\alpha| - 1 \leq t \leq \frac{1}{3}$$

On the other hand, the positivity region for  $\rho_2$  is given by the conditions

$$-\frac{1}{3} \leq t \leq 1 \quad \text{and} \quad |\alpha| \leq \frac{1}{2} \sqrt{1 + 2t - 3t^2}$$

## 5 Critical points of the mapping $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$

### 5.1 Formulation of the problem

In this section we start to analyze the real problem of finding minimum of the trace norm  $\|S(\mathcal{M})\|_1$  in general case. As a first step, we will study critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ . Since the projector  $\mathcal{P} = \mathbb{1}_3 - \mathcal{M}$  is one dimensional, there is a unit vector  $v \in \mathbb{R}^3$  such that  $\mathcal{P} = P_v$ . The vector  $v$  is given by the third column of the matrix  $V \in \text{SO}(3)$  relating  $\mathcal{P}$  and  $\mathcal{P}_0$  (2.9). To study critical points of trace norm of disturbance, it is useful to consider the auxiliary function  $\mathbf{g}$  defined on the unit sphere  $\mathbb{S}^2 \subset \mathbb{R}^3$  with values in  $\mathbb{R}^2$ . The function is defined as follows:

$$\mathbf{g}(v) = (g_1(v), g_2(v)) \tag{5.1}$$

where

$$g_1(v) = \|(\mathbb{1}_3 - P_v)x\|^2 + \text{tr}((\mathbb{1}_3 - P_v)KK^T) \tag{5.2}$$

and

$$g_2(v) = 4 \left( \|K^T(\mathbb{1}_3 - P_v)x\|^2 + \text{tr}(E^T E P_v) \right) \tag{5.3}$$

Notice that using the functions (5.2) and (5.3), the formula (3.1) can be rewritten as

$$\|S(\mathcal{M})\|_1 = \|S(\mathbb{1}_3 - P_v)\|_1 = \frac{1}{\sqrt{2}} \sqrt{g_1(v) + \sqrt{g_1(v)^2 - g_2(v)}}$$

In the following we will consider the mapping  $\mathbf{g}$  as a function of two-dimensional projectors  $\mathcal{M}$  or vectors  $v \in \mathbb{S}^2$ .

The formulas (5.2) and (5.3) can be further simplified if we introduce the following operators

$$W_y z = \langle z, y \rangle y, \quad y, z \in \mathbb{R}^3 \tag{5.4}$$

and

$$L_+ = K K^T + W_x \tag{5.5}$$

where  $x$  is a Bloch vector. Now we obtain

$$g_1(v) = \|x\|^2 - \langle x, v \rangle^2 + \text{tr}(K K^T) - \langle v, K K^T v \rangle = \text{tr} L_+ - \langle v, L_+ v \rangle \tag{5.6}$$

and

$$g_2(v) = 4 \left( \|K^T(x - \langle x, v \rangle x)\|^2 + \langle v, E^T E v \rangle \right) \tag{5.7}$$

From Eq. (5.6) we obtain, in particular, that

$$\min_{v \in \mathbb{S}^2} g_1(v) = \text{tr} L_+ - \lambda_3 = \lambda_1 + \lambda_2 \tag{5.8}$$

where  $\lambda_1 \leq \lambda_2 \leq \lambda_3$  are the eigenvalues of real nonnegative matrix  $L_+$ . The relation (5.8) allows to obtain the first general result concerning the value of geometric discord  $D_1(\rho)$ . Namely we have

**Theorem 5.1** *For any two-qubit state (2.3) we have*

$$D_1(\rho) \geq \frac{1}{\sqrt{2}} \sqrt{\lambda_1 + \lambda_2} \tag{5.9}$$

where  $\lambda_1 \leq \lambda_2 \leq \lambda_3$  are the eigenvalues of  $L_+ = K K^T + W_x$ .

From the relation (5.8) we can also derive well-known exact formula for Hilbert–Schmidt norm geometric discord  $D_2(\rho)$  [5]. By definition

$$D_2(\rho) = \min_{\mathcal{M}} 2 \text{tr} Q(\mathcal{M})$$

Using (3.2) we obtain

$$\text{tr} Q(\mathcal{M}) = \frac{1}{4} \left( \text{tr}(\mathcal{M} K K^T) + \langle \mathcal{M} x, x \rangle \right) = \frac{1}{4} g_1(v)$$

so

$$D_2(\rho) = \min_{v \in \mathbb{S}^2} \frac{1}{2} g_1(v) = \frac{1}{2} (\lambda_1 + \lambda_2)$$

Obviously, for any two-qubit state

$$D_1(\rho) \geq \sqrt{D_2(\rho)}$$

The right-hand side of (5.9) in some cases gives not only the lower bound but the exact value of discord  $D_1$ . It can happen for such states  $\rho$  for which  $D_1(\rho) = \sqrt{D_2(\rho)}$ . Below we show it for an explicit family of states. Consider the states [11]

$$\rho_\theta = \frac{1}{4} \begin{pmatrix} 2 \cos^2 \theta & 0 & 0 & \sin 2\theta \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ \sin 2\theta & 0 & 0 & 2 \sin^2 \theta \end{pmatrix}, \quad \theta \in [0, \pi/2] \quad (5.10)$$

For the family (5.10), we have

$$x = \begin{pmatrix} 0 \\ 0 \\ -\sin^2 \theta \end{pmatrix}, \quad y = \begin{pmatrix} 0 \\ 0 \\ \cos^2 \theta \end{pmatrix}$$

and

$$K = \text{diag}(\cos \theta \sin \theta, -\cos \theta \sin \theta, 0)$$

so

$$K K^T + W_x = \text{diag}(\cos^2 \theta \sin^2 \theta, \cos^2 \theta \sin^2 \theta, \sin^4 \theta) \quad (5.11)$$

The order of eigenvalues of (5.11) depends on  $\theta$ . For  $\theta \in [0, \pi/4]$

$$\sin^4 \theta \leq \sin^2 \theta \cos^2 \theta$$

and for such  $\theta$

$$\frac{1}{\sqrt{2}} \sqrt{\lambda_1 + \lambda_2} = \frac{1}{\sqrt{2}} \sqrt{\sin^4 \theta + \sin^2 \theta \cos^2 \theta} = \frac{1}{\sqrt{2}} \sin \theta$$

On the other hand, one can check that

$$D_1(\rho_\theta) = \frac{1}{2} \sin 2\theta \geq \frac{1}{\sqrt{2}} \sin \theta$$

so in this case we obtain only the lower bound. Now for  $\theta \in (\pi/4, \pi/2]$

$$\sin^2 \theta \cos^2 \theta \leq \sin^4 \theta$$

and for such  $\theta$

$$\frac{1}{\sqrt{2}}\sqrt{\lambda_1 + \lambda_2} = \frac{1}{\sqrt{2}}\sqrt{2 \sin^2 \theta \cos^2 \theta} = \sin \theta \cos \theta = \frac{1}{2} \sin 2\theta$$

which equals to the value of  $D_1(\rho_\theta)$ .

### 5.2 Singular critical points

We see that the problem of finding minimum of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  is relatively easy when it is achieved on the set

$$\mathbb{D} = \{v \in \mathbb{S}^2 : g_1^2(v) = g_2(v)\} \tag{5.12}$$

Each critical point  $v_0 \in \mathbb{D}$  is called a *singular critical point* in contrast to the *smooth critical point*, i.e., critical point belonging to the set  $\mathbb{S}^2 \setminus \mathbb{D}$ . When the minimum is achieved at some singular critical point, the minimal value of trace norm  $\|S(\mathcal{M})\|_1$  is given by the minimum of the function  $g_1$ . To study the properties of the set  $\mathbb{D}$ , consider another representations of the functions  $g_1$  and  $g_2$ . Let  $L_- = KK^T - W_x$ . One can check that

$$g_1(v) = \text{tr } L_- - \langle v, L_- v \rangle + 2(\|x\|^2 - \langle x, v \rangle^2) \tag{5.13}$$

and

$$g_2(v) = 4(\|x\|^2 - \langle x, v \rangle^2) \left[ \text{tr } L_- - \langle v, L_- v \rangle + \|x\|^2 - \langle x, v \rangle^2 \right] + 4\langle v, \text{adj } L_- v \rangle \tag{5.14}$$

where we dropped the term proportional to  $1 - \|v\|^2$ . Using (5.13) and (5.14) one can show that the set (5.12) can be discrete or it can be equal to the whole sphere  $\mathbb{S}^2$ . It follows from the following lemma, which can be proved by a direct computation.

**Lemma 5.1** *Let  $\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3$  be the eigenvalues of the matrix  $L_-$ . The vectors  $v \in \mathbb{D}$  satisfy*

$$(\tilde{\lambda}_1 - \tilde{\lambda}_2)^2 (v_3^2 - v_1^2 v_2^2) + (\tilde{\lambda}_2 - \tilde{\lambda}_3)^2 (v_1^2 - v_2^2 v_3^2) + (\tilde{\lambda}_1 - \tilde{\lambda}_3)^2 (v_2^2 - v_1^2 v_3^2) = 0 \tag{5.15}$$

**Remark 5.1** One can check that in the discrete case, the set  $\mathbb{D}$  can contain only one or two projectors, if we identify the vectors  $v$  and  $-v$ .

For the further analysis it is crucial to have a convenient criterion that enables to decide whether the value of  $D_1(\rho)$  is achieved at a critical point belonging to the set  $\mathbb{D}$  or  $\mathbb{S}^2 \setminus \mathbb{D}$ . To obtain such criterion, consider the function

$$F(t, s) = t + \sqrt{t^2 - s}$$

defined on the region

$$\Omega = \{(t, s) \in \mathbb{R}^2; t \geq 0, s \geq 0, t^2 \geq s\}$$

For any  $t_* > 0$  consider the function

$$\delta_{t_*}(t) = \begin{cases} t^2, & t \geq t_* \\ 2t_*t - t_*^2, & t_*/2 \leq t \leq t_* \end{cases}$$

And finally, define the family of regions  $\Omega_{t_*}, t_* \geq 0$  such that  $\Omega_0 = \Omega$  and for  $t_* > 0$

$$\Omega_{t_*} = \{(t, s) \in \mathbb{R}^2; t \geq 0, s \geq 0, \delta_{t_*}(t) \geq s\}$$

Suppose now that the function  $g_1$  restricted to  $\mathbb{D}$  achieves at some vector  $v_* \in \mathbb{D}$  its absolute minimum. Let  $\text{Ran } \mathbf{g}$  be the range of the function  $\mathbf{g}$ . The values of  $D_1(\rho)$  are achieved at  $v_* \in \mathbb{D}$  if and only if

$$\text{Ran } \mathbf{g} \subset \Omega_{g_1(v_*)}$$

So we obtain

**Proposition 5.1** *Let the function  $g_1$  restricted to  $\mathbb{D}$  achieve its absolute minimum at the vector  $v_* \in \mathbb{D}$ . The value of  $D_1(\rho)$  is achieved at this vector, if and only if the following conditions are satisfied*

$$g_1(v_*) \leq 2g_1(v) \tag{5.16}$$

for all  $v \in \mathbb{S}^2$ , and

$$g_1(v_*)g_1(v) \geq \frac{1}{2}(g_2(v) + g_2(v_*)) \tag{5.17}$$

for all  $v \in \mathbb{S}^2$  such that  $g_1(v) \leq g_1(v_*)$ .

**Remark 5.2** Notice that if the conditions (5.16) and (5.17) are not satisfied, then the value  $g_1(v_*)$  gives the upper bound for  $D_1(\rho)$ , i.e.,

$$D_1(\rho) \leq \frac{1}{\sqrt{2}} \sqrt{g_1(v_*)}$$

Now we determine the minimal value  $g_1(v_*)$ . To this end, consider the following cases:

- $\tilde{\lambda}_1 > \tilde{\lambda}_2 > \tilde{\lambda}_3$ . The solutions of (5.15) are given by

$$v_1^2 = \frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_1 - \tilde{\lambda}_3}, \quad v_1^2 = 0, \quad v_3^2 = \frac{\tilde{\lambda}_2 - \tilde{\lambda}_3}{\tilde{\lambda}_1 - \tilde{\lambda}_3} \tag{5.18}$$

and the expression for  $g_1(v)$ ,  $v \in \mathbb{D}$  reads

$$g_1(v) = 2 \left( \tilde{\lambda}_2 + \|x\|^2 - \langle x, v \rangle^2 \right) \tag{5.19}$$

Note that  $\tilde{\lambda}_2 \geq 0$ . The equality (5.19) is valid in any orthonormal basis. But if we choose the basis of ordered and normalized eigenvectors of  $L_-$ , then

$$g_1(v_*) = 2 \left( \tilde{\lambda}_2 + \frac{1}{\tilde{\lambda}_1 - \tilde{\lambda}_3} \left[ (\tilde{\lambda}_1 - \tilde{\lambda}_3)x_2^2 + \left( \sqrt{\tilde{\lambda}_2 - \tilde{\lambda}_3} |x_1| - \sqrt{\tilde{\lambda}_1 - \tilde{\lambda}_2} |x_3| \right)^2 \right] \right)$$

- 2.  $\tilde{\lambda}_1 = \tilde{\lambda}_2 > \tilde{\lambda}_3$ . Equation (5.15) gives  $v_1 = v_2 = 0$  and  $v_3^2 = 1$ . So (5.19) is also valid and we obtain

$$g_1(v_*) = 2 (\tilde{\lambda}_2 + x_1^2 + x_2^2)$$

- 3.  $\tilde{\lambda}_1 = \tilde{\lambda}_2 = \tilde{\lambda}_3$ . In this case  $\mathbb{D} = \mathbb{S}^2$  and the formula (5.19) is valid.

So we have the following

**Proposition 5.2** *For all vectors  $v \in \mathbb{D}$*

$$g_1(v) = 2 \left( \text{int}\{\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3\} + \|x\|^2 - \langle x, v \rangle^2 \right) \tag{5.20}$$

where *int* denotes the intermediate value and  $\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3$  are the eigenvalues of the matrix  $L_-$ .

**Remark 5.3** Notice that if the Bloch vector  $x$  is zero vector, then the function  $g_1$  is constant on the set  $\mathbb{D}$  and equals to  $2 \text{int}\{\lambda_1, \lambda_2, \lambda_3\}$ , where  $\lambda_1, \lambda_2, \lambda_2$  are the eigenvalues of the matrix  $KK^T$ .

### 5.3 Smooth critical points

Smooth critical points  $v_0 \in \mathbb{S}^2 \setminus \mathbb{D}$  satisfy

$$g_1^2(v_0) \neq g_2(v_0)$$

Applying differential analysis to the set  $\mathbb{S}^2 \setminus \mathbb{D}$  one can find all smooth critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ . Let

$$f^2 = g_1 + \sqrt{g_1^2 - g_2} - \lambda (1 - \|v\|^2)$$



with the constrain  $\|v\| = 1$  and where  $\lambda$  is a Lagrange multiplier. For the smooth critical points one obtains

$$4\mu \operatorname{grad} g_1 - \operatorname{grad} g_2 = -8\omega v \tag{5.21}$$

where  $2\omega = \lambda \sqrt{g_1^2 - g_2}$ . Moreover,  $4\mu = 2f^2$ , i.e.,

$$\|S(\mathcal{M})\|_1 = \sqrt{\mu} \tag{5.22}$$

**Remark 5.4** The condition (5.21), in particular, means that smooth critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  are critical points of the function  $\mathbf{g}$  defined by (5.1).

To find critical points of  $\mathbf{g}$  we look for the possible solutions of the equation

$$\left[ W_x P_v K K^T + K K^T P_v W_x - K K^T W_x - W_x K K^T + E^T E + \mu L_+ \right] v = \omega v \tag{5.23}$$

A vector  $v \in \mathbb{S}^2$  is a solution of (5.23) if there exists a real number  $\mu$  such that  $v$  is a solution of the above eigenvector problem. Applying the above results one can prove the following theorem:

**Theorem 5.2** Any smooth critical point of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  satisfies (5.23), i.e., is a critical point of the function  $\mathbf{g}$ .

**Remark 5.5** One can also show that critical points contained in the set  $\mathbb{D}$  satisfy (5.23), so the thesis of Theorem 5.2 is true for all critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ .

The condition in Eq. (5.23) can be rewritten in the following way. Notice that the two-dimensional projector  $\mathcal{M}$  is a critical point of the function  $\mathbf{g}$  if and only if it commutes with the matrix

$$G_\mu = -W_x \mathcal{M} K K^T - K K^T \mathcal{M} W_x + E^T E + \mu L_+ \tag{5.24}$$

i.e.,  $v$  is the solution of (5.23) if and only if

$$G_\mu P_v = P_v G_\mu \tag{5.25}$$

On the other hand, the information about the Lagrange multiplier  $\omega$  can be recovered from Eq. (5.25) that leads to

$$G_\mu P_v = \omega P_v \tag{5.26}$$

### 5.4 First application: states with maximally mixed marginals

General analysis of Eqs. (5.23) or (5.25) will be presented in the next section; here we consider the first application to the states with maximally mixed marginals (MMM states), i.e., such states  $\rho$  that

$$\text{tr}_{\mathcal{A}}\rho = \text{tr}_{\mathcal{B}}\rho = \frac{1}{2}\mathbb{1}_2$$

In this case the Bloch vectors  $x$  and  $y$  are zero vectors. Let  $K$  be the correlation matrix of MMM state  $\rho$ . Using the local transformation one can bring the matrix  $KK^T$  to the diagonal form  $\text{diag}(i_1^2, i_2^2, i_3^2)$  with  $i_1^2 \geq i_2^2 \geq i_3^2$ . Now Eq. (5.15) for the set  $\mathbb{D}$  has a form

$$(i_1^2 - i_2^2)^2 (v_3^2 - v_1^2 v_2^2) + (i_2^2 - i_3^2)^2 (v_1^2 - v_2^2 v_3^2) + (i_1^2 - i_3^2)^2 (v_2^2 - v_1^2 v_3^2) = 0 \tag{5.27}$$

Moreover

$$G_\mu = E^T E + \mu K K^T = \text{diag}(i_2^2 i_3^2 + \mu i_1^2, i_1^2 i_3^2 + \mu i_2^2, i_1^2 i_2^2 + \mu i_3^2) \tag{5.28}$$

so the general form of  $P_v$  satisfying (5.26) depends on the degeneracy of the eigenvalues of  $G_\mu$ .

Consider first the case when  $i_1^2 > i_2^2 > i_3^2$ . Suppose that  $\mu \notin \{i_1^2, i_2^2, i_3^2\}$ , then the eigenvalues of  $G_\mu$  are non-degenerate and the only possible solutions of (5.26) correspond to the vectors

$$(1, 0, 0), \quad (0, 1, 0) \quad \text{and} \quad (0, 0, 1)$$

which, according to (5.27) cannot belong to the set  $\mathbb{D}$ . So they can be smooth critical points of  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ . The condition (5.22) enforces  $\mu = i_1^2$  or  $\mu = i_2^2$ , which is in a contradiction with the assumption that  $\mu \notin \{i_1^2, i_2^2, i_3^2\}$ . So we conclude that the square of the discord can be achieved in the set  $\mu \in \{i_1^2, i_2^2\}$ , since  $i_3^2$  can be excluded because of the lower bound given by Theorem 5.1

$$2\mu \geq i_2^2 + i_3^2$$

Since  $i_2^2 < i_1^2$ , we get

$$D_1(\rho) = \text{int}\{|i_1|, |i_2|, |i_3|\} \tag{5.29}$$

Similarly, one also obtains the formula (5.29) in the case when  $i_1^2 = i_2^2 > i_3^2$  or  $i_1^2 > i_2^2 = i_3^2$ . The case  $i_1^2 = i_2^2 = i_3^2$  is trivial: The set  $\mathbb{D}$  is equal to the whole sphere  $\mathbb{S}^2$ , the function (5.22) is constant, and we again obtain (5.29). Thus, we confirm the known result (see, e.g., [9])

**Conclusion 5.1** *For any MMM state trace-norm geometric discord is equal to the intermediate value in the set of singular values of the corresponding correlation matrix.*

### 6 Main result: determination of quantum discord in general case

In this section we use Eq. (5.25) to solve the main problem, namely to find the value of geometric discord in general case. It is convenient to consider the matrix (5.24) with respect to ordered basis of orthonormal eigenvectors of the operator  $L_-$ . (We will assume that  $\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \tilde{\lambda}_3$ .) When we also neglect the parts which commute with the projectors  $P_v$ , we obtain the matrix

$$\tilde{G}_\mu = W_x P_v \Lambda + \Lambda P_v W_x + 2 P_x W_v P_x - (\tilde{\lambda}_1 - \tilde{\lambda}_2) W_x + \tilde{\mu}(\Lambda + 2 W_x) + (\tilde{\lambda}_1 - \tilde{\lambda}_2)(\tilde{\lambda}_2 - \tilde{\lambda}_3) P_{y_0}$$

where

$$\Lambda = \begin{pmatrix} \tilde{\lambda}_1 - \tilde{\lambda}_3 & 0 & 0 \\ 0 & \tilde{\lambda}_2 - \tilde{\lambda}_3 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad y_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

and

$$\tilde{\mu} = \mu - \tilde{\lambda}_2 - \|x\|^2$$

In the following we will also use the matrices  $\tilde{\Lambda} = \Lambda - (\tilde{\lambda}_1 - \tilde{\lambda}_2) \mathbb{1}_3$  and

$$\Pi = \begin{pmatrix} 0 & (\tilde{\lambda}_1 - \tilde{\lambda}_2)x_3 & -(\tilde{\lambda}_1 - \tilde{\lambda}_3)x_2 \\ (\tilde{\lambda}_1 - \tilde{\lambda}_2)x_3 & 0 & (\tilde{\lambda}_2 - \tilde{\lambda}_3)x_1 \\ -(\tilde{\lambda}_1 - \tilde{\lambda}_3)x_2 & (\tilde{\lambda}_2 - \tilde{\lambda}_3)x_1 & 0 \end{pmatrix}$$

Notice that if  $L_-$  has a degenerate spectrum, the form of the operator  $\tilde{G}_\mu$  is particularly simple and the desired minimal value of  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  can be found in a straightforward way.

#### 6.1 Non-degenerate spectrum of $L_-$

Assume that  $\tilde{\lambda}_1 > \tilde{\lambda}_2 > \tilde{\lambda}_3$ . First, we find the location of critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ . Notice that in the following all components of the vector  $v$  and the Bloch vector  $x$  are computed with respect to the ordered basis of orthonormal eigenvectors of  $L_-$ .

**Proposition 6.1** *Assume that the matrix  $L_- = K K^T - W_x$  has non-degenerate eigenvalues. The critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  ( $\mathcal{M} = \mathbb{1}_3 - P_v$ ) are contained in the subset of vectors  $v \in \mathbb{S}^2$  satisfying the condition*

$$v_1 v_2 v_3 = 0$$

*i.e., in the big circles in  $\mathbb{S}^2$ , where the components of  $v$  are given with respect to the ordered basis of eigenvectors of  $L_-$ . In particular, the value of  $D_1(\rho)$  is achieved only on such vectors.*

**Proof** Suppose that critical points do not satisfy the condition  $v_1 v_2 v_3 = 0$  and moreover let  $v_3 x_1 - v_1 x_3 \neq 0$ . The condition  $v_1 v_2 v_3 \neq 0$  implies that the critical points are outside the set  $\mathbb{D}$ . Notice that  $\tilde{\mu} + \langle x, v \rangle^2 \geq 0$ . Since (5.25) is satisfied, the following strict inequality is true

$$\tilde{\mu} + \langle x, v \rangle^2 > 0$$

By a direct computation one can find the representation of  $\tilde{\mu}$

$$(\tilde{\mu} + \langle x, v \rangle^2)(v_3 x_1 - v_1 x_3) = -(v_3 x_1 - v_1 x_3)\langle v, \tilde{\Lambda} v \rangle - \frac{1}{2} v_2 \langle v, \Pi v \rangle$$

along the critical points of the function  $\mathbf{g}$ , described by the condition

$$v_2 \langle v, \Pi v \rangle + (v_3 x_1 - v_1 x_3)\langle v, \tilde{\Lambda} v \rangle = 0 \tag{6.1}$$

or

$$\langle x, v \rangle(v_3 x_1 - v_1 x_3) + (\tilde{\lambda}_1 - \tilde{\lambda}_3)v_1 v_3 = 0 \tag{6.2}$$

To find the critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  we use the condition (5.22), which now reads

$$\begin{aligned} &4(\tilde{\lambda}_1 - \tilde{\lambda}_2)(\tilde{\lambda}_2 - \tilde{\lambda}_3)(v_3 x_1 - v_1 x_3)^2 v_2 \\ &= \langle v, \Pi v \rangle(v_2 \langle v, \Pi v \rangle + 2(v_3 x_1 - v_1 x_3)\langle v, \tilde{\Lambda} v \rangle) \end{aligned}$$

To obtain the result, let us assume that Eq. (6.1) has a non-empty set of solutions. Then, we get that

$$2\tilde{\mu} = -2\langle x, v \rangle^2 - \langle v, \tilde{\Lambda} v \rangle$$

But this representation can not be valid outside the set  $\mathbb{D}$  and we obtain the contradiction with our assumption. Let now Eq. (6.2) has the non-empty set of solutions. Then, we get

$$(\tilde{\lambda}_1 - \tilde{\lambda}_3)(\tilde{\mu} + \langle x, v \rangle^2)v_1 v_3 = (\tilde{\lambda}_1 - \tilde{\lambda}_3)v_1 v_3(2(\tilde{\mu} + \langle x, v \rangle^2) + \langle v, \tilde{\Lambda} v \rangle)$$

and after simplifications we obtain

$$\tilde{\mu} = -\langle x, v \rangle^2 - \langle v, \tilde{\Lambda} v \rangle$$

But this is impossible, as this leads to the condition  $v_2 = 0$ . Finally, let  $v_3 x_1 - v_1 x_3 = 0$ . Then, Eq. (5.25) gives

$$\tilde{\mu} + \langle x, v \rangle^2 = 0$$

This condition together with (5.22) leads again to  $v_2 = 0$ . □

The assumption of non-degeneracy of the spectrum of  $L_-$  is relevant in the above result. On the other hand, the proof suggests that the location of critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  given by Proposition 6.1 is not optimal. Indeed, if, for example,  $x_1 \neq 0$ , the critical points cannot satisfy  $v_1 = 0$  if  $v_2 v_3 \neq 0$ . Similarly, if  $x_3 \neq 0$ , the critical points never lay on the big circle  $v_3 = 0$  with  $v_1 v_2 \neq 0$ , unless  $\tilde{\lambda}_1 + \tilde{\lambda}_3 > 2\tilde{\lambda}_2$  and the following condition is satisfied

$$x_1^2 + x_2^2 = \frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_2 - \tilde{\lambda}_3} x_1^2$$

The additional information of this kind can simplify the determination of quantum discord in some situations. Nevertheless, we will not discuss this improvements here and focus on the direct method of finding the absolute minimum of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ .

Now we can go to the solution of the main problem. This is a problem of minimizing the quadratic form  $\mu$ , restricted to the big circles. The calculations are elementary but tedious, so we do not present all details.

1. Let us start with  $v_1 = 0$ . One can find

$$\tilde{\mu} = \tilde{\lambda}_1 - \tilde{\lambda}_2 - \langle x, v \rangle^2$$

and

$$\tilde{\mu}_{\min} = \tilde{\lambda}_1 - \tilde{\lambda}_2 - \|x\|^2 + x_1^2$$

So

$$D_1(\rho)^2 \leq \tilde{\lambda}_1 + x_1^2$$

2. Let  $v_3 = 0$ . Then

$$\tilde{\mu} = (\tilde{\lambda}_1 - \tilde{\lambda}_2)v_2^2 - \langle x, v \rangle^2$$

Inserting the minimum  $\tilde{\mu}_{\min}$  one gets

$$D_1(\rho) \leq \frac{1}{\sqrt{2}} \sqrt{\tilde{\lambda}_1 + \tilde{\lambda}_2 + \|x\|^2 + x_3^2 - \sqrt{(\tilde{\lambda}_1 - \tilde{\lambda}_2 + \|x\|^2 - x_3^2)^2 - 4(\tilde{\lambda}_1 - \tilde{\lambda}_2)x_2^2}}$$

3. Let finally  $v_2 = 0$ . This case is not so straightforward. One needs to introduce the additional parameter. We start with the formula

$$2\tilde{\mu} = \tilde{\lambda}_1 - \tilde{\lambda}_2 - (\tilde{\lambda}_1 - \tilde{\lambda}_3)v_1^2 + |\tilde{\lambda}_1 - \tilde{\lambda}_2 - (\tilde{\lambda}_1 - \tilde{\lambda}_3)v_1^2| - 2\langle x, v \rangle^2 \quad (6.3)$$

To describe the absolute minimum of the function (6.3), we need to consider auxiliary functions. The complexity of formulae below mainly follows from the presence of the absolute value in (6.3). Let us define functions  $p(\theta)$  and  $r(\theta)$ , as follows: The common

domain of  $p(\theta)$  and  $r(\theta)$  is the closed interval  $[-\pi, \pi]$ . To define these functions we need the gap angle  $\varphi_{\text{gap}} \in (0, \pi/2)$ , determined by the equation

$$\cos \varphi_{\text{gap}} = \sqrt{\frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_1 - \tilde{\lambda}_3}}$$

Moreover, let  $\sigma : [-\pi, \pi] \rightarrow [-1, 1]$  be any function such that

$$\sigma(\theta) = \begin{cases} 1, & \theta \in (-\pi, -\pi/2) \cup (0, \pi/2) \\ -1, & \theta \in (-\pi/2, 0) \cup (\pi/2, \pi) \end{cases}$$

and  $\mathcal{O}_{\text{gap}}$  be the open set

$$\mathcal{O}_{\text{gap}} = (-\pi + \varphi_{\text{gap}}, -\varphi_{\text{gap}}) \cup (\varphi_{\text{gap}}, \pi - \varphi_{\text{gap}})$$

Now we are ready to define

$$p(\theta) = \begin{cases} 1, & \theta \in \mathcal{O}_{\text{gap}} \\ \cos^2(\theta - \sigma(\theta) \varphi_{\text{gap}}), & \theta \in [-\pi, \pi] \setminus \mathcal{O}_{\text{gap}} \end{cases}$$

and

$$r(\theta) = \begin{cases} \cos^2(\theta - \sigma(\theta) \varphi_{\text{gap}}), & \theta \in \mathcal{O}_{\text{gap}} \\ 1, & \theta \in [-\pi, \pi] \setminus \mathcal{O}_{\text{gap}} \end{cases}$$

Finally, let  $\theta_*$  and  $\theta_{**}$  be the angles defined below in two steps. First, let  $x_1 x_3 \neq 0$ . Define

$$\begin{aligned} \cos \theta_* &= \frac{\sqrt{2}|x_1 x_3|}{\sqrt{N_*(N_* - \tilde{\lambda}_1 + \tilde{\lambda}_3 - x_1^2 + x_3^2)}}, \\ \sin \theta_* &= -\frac{\sqrt{2}x_1 x_3}{\sqrt{N_*(N_* + \tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 - x_3^2)}} \end{aligned} \tag{6.4}$$

where

$$N_* = \sqrt{(\tilde{\lambda}_1 - \tilde{\lambda}_3 + \|x\|^2 - x_2^2)^2 - 4(\tilde{\lambda}_1 - \tilde{\lambda}_3)x_3^2}$$

and

$$\cos \theta_{**} = \frac{\sqrt{2}|x_1 x_3|}{\sqrt{N_{**}(N_{**} - x_1^2 + x_3^2)}}, \quad \sin \theta_{**} = -\frac{\sqrt{2}x_1 x_3}{\sqrt{N_{**}(N_{**} + x_1^2 - x_3^2)}} \tag{6.5}$$

with

$$N_{**} = \|x\|^2 - x_2^2$$

If  $x_1x_3 = 0$ , we pass to the one-sided limits  $x_1 \rightarrow 0^\pm$  or  $x_3 \rightarrow 0^\pm$  (or both) in the formulas (6.4) and (6.5). The left and right limits can only differ by sign, but this has no importance as the functions  $p(\theta)$  and  $r(\theta)$  give the same result in these situations.

To obtain the upper bound for quantum discord, define

$$\mu_* = \frac{1}{2} \left( \tilde{\lambda}_1 + \tilde{\lambda}_3 + \|x\|^2 + x_2^2 + N_*(1 - 2p(\theta_*)) \right) \tag{6.6}$$

and

$$\mu_{**} = \tilde{\lambda}_2 + \|x\|^2 - (\|x\|^2 - x_2^2)r(\theta_{**}) \tag{6.7}$$

Then, one can show that

$$D_1(\rho) \leq \sqrt{\min\{\mu_*, \mu_{**}\}}$$

The above analysis leads to the following result.

**Theorem 6.1** *In the case of non-degenerate spectrum of the matrix  $KK^T - W_x$ , the value of trace-norm geometric discord is given by*

$$D_1(\rho) = \sqrt{\min\{d_1, d_2, d_3\}}$$

where

$$\begin{aligned} d_1 &= \tilde{\lambda}_1 + x_1^2, \\ d_2 &= \frac{1}{2} \left( \tilde{\lambda}_1 + \tilde{\lambda}_2 + \|x\|^2 + x_3^2 - \sqrt{(\tilde{\lambda}_1 - \tilde{\lambda}_2 + \|x\|^2 - x_3^2)^2 - 4(\tilde{\lambda}_1 - \tilde{\lambda}_2)x_2^2} \right), \\ d_3 &= \min\{\mu_*, \mu_{**}\} \end{aligned}$$

with  $\mu_*, \mu_{**}$  given by (6.6) and (6.7), respectively.

### 6.2 Degenerate spectrum of $L_-$

When there is any degeneracy in the spectrum of  $L_-$ , the analysis simplifies significantly. From the above discussion we obtain:

**Theorem 6.2** 1. *Let  $\tilde{\lambda}_1 = \tilde{\lambda}_2 \geq \tilde{\lambda}_3$ , then*

$$D_1(\rho) = \sqrt{\tilde{\lambda}_2}$$

2. *Let  $\tilde{\lambda}_1 > \tilde{\lambda}_2 = \tilde{\lambda}_3$ , then*

$$D_1(\rho) = \frac{1}{\sqrt{2}} \sqrt{\tilde{\lambda}_1 + \tilde{\lambda}_2 + \|x\|^2 - \sqrt{(\tilde{\lambda}_1 - \tilde{\lambda}_2 + \|x\|^2)^2 + 4(\tilde{\lambda}_1 - \tilde{\lambda}_2)x_1^2}}$$

## 7 Examples

In this section we present the applications of Theorems 6.1 and 6.2 to the cases already known in the literature as well as to the new examples of states. But we start with considering again, from the wider perspective, the results obtained in Sects. 4 and 5.4.

### 7.1 The class $\mathcal{E}_0$

In this case the correlation matrix is of the form  $K = t V_0$ , where  $V_0$  is orthogonal and the Bloch vectors  $x$  and  $y$  are arbitrary. Thus

$$L_- = t^2 \mathbb{1}_3 - \|x\|^2 P_x$$

and

$$\text{spect } L_- = \{t^2, t^2, t^2 - \|x\|^2\}$$

So we can apply Theorem 6.2 to obtain

$$D_1(\rho) = |t|$$

### 7.2 The class of MMM states

In this case Bloch vectors  $x$  and  $y$  are zero vectors, so

$$L_- = K K^T$$

Let  $\lambda_1 \geq \lambda_2 \geq \lambda_3$  be the eigenvalues of  $K K^T$ . When the eigenvalues are degenerate, we apply Theorem 6.2 and obtain  $D_1(\rho) = \sqrt{\lambda_2}$ . In the non-degenerate case we must apply Theorem 6.1 and the computation is more involved. Observe that in the case of MMM states

$$d_1 = \lambda_1, \quad d_2 = \lambda_2, \quad d_3 = \min\{\mu_*, \mu_{**}\}$$

where obviously  $\mu_{**} = \lambda_2$ . To show that  $\mu_*$  also equals to  $\lambda_2$  one checks that  $\theta_* = 0$ . Then

$$p(\theta_*) = \cos^2 \varphi_{\text{gap}} = \frac{\lambda_1 - \lambda_2}{\lambda_1 - \lambda_3}$$

so by (6.6),  $\mu_* = \lambda_2$ . Thus

$$D_1(\rho) = \min\{d_1, d_2, d_3\} = \sqrt{\lambda_2}$$



### 7.3 Pure states

It is well known that up to the local equivalence, every pure state has the form

$$\rho_N = \frac{1}{2} \begin{pmatrix} 1 + \sqrt{1 - N^2} & 0 & 0 & N \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ N & 0 & 0 & 1 - \sqrt{1 - N^2} \end{pmatrix}, \quad N \in [0, 1] \quad (7.1)$$

The corresponding correlation matrix and Bloch vector are given by

$$K = \begin{pmatrix} N & 0 & 0 \\ 0 & -N & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad x = \begin{pmatrix} 0 \\ 0 \\ \sqrt{1 - N^2} \end{pmatrix}$$

So

$$L_- = \begin{pmatrix} N^2 & 0 & 0 \\ 0 & N^2 & 0 \\ 0 & 0 & N^2 \end{pmatrix}$$

an we can apply Theorem 6.2 to obtain

$$D_1(\rho_N) = N$$

On the other hand, the measure of entanglement defined by negativity gives the same value.

### 7.4 X-states

Two-qubit X-state has the X-shaped form

$$\rho_X = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix} \quad (7.2)$$

We can always take off-diagonal matrix elements  $\rho_{14}$  and  $\rho_{23}$  to be positive [10]. Then, the correlation matrix  $K$  is diagonal and the Bloch vector  $x$  has only third component nonzero. So the matrix  $KK^T$  is diagonal and commutes with the operator  $W_x$ . It follows that the matrix  $L_-$  has also diagonal form and the basis of eigenvector of  $L_-$  coincides with the canonical basis. Since the spectrum of  $L_-$  is in general non-degenerate, to find the value of  $D_1(\rho_X)$  we apply Theorem 6.1. Let us start with computing  $\mu_*$  and  $\mu_{**}$ . Notice that this case when  $x_1 x_3 = 0$  as  $x_1 = x_2 = 0$ . Let

$$n_* = \tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 - x_3^2$$

then

$$\cos \theta = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{n_*}{\sqrt{n_*^2 + 4x_1^2 x_3^2}}} \quad \text{and} \quad \cos \theta_* = \lim_{x_1 \rightarrow 0} \cos \theta$$

We can choose the sign of  $x_1$  such that  $\sin \theta > 0$ , so the angles are in the interval  $[0, \pi/2]$ . Computing this limit we obtain:

- for  $\tilde{\lambda}_1 > \tilde{\lambda}_3 + ||x||^2$ ,  $\theta_* = 0$ , then  $N_* = \tilde{\lambda}_1 - \tilde{\lambda}_3 - ||x||^2$ ,  $\sigma(\theta_*) = \pm 1$
- for  $\tilde{\lambda}_1 = \tilde{\lambda}_3 + ||x||^2$ ,  $\theta_* = \pi/4$ , then  $N_* = 0$
- for  $\tilde{\lambda}_1 < \tilde{\lambda}_3 + ||x||^2$ ,  $\theta_* = \pi/2$ , then  $N_* = \tilde{\lambda}_3 + ||x||^2 - \tilde{\lambda}_1$ ,  $\sigma(\theta_*) = \pm 1$ .

Let  $\theta_* = 0$ , then  $p(0) = \cos^2(0 \pm \varphi_{\text{gap}}) = \cos^2(\varphi_{\text{gap}})$ , so

$$\mu_* = \tilde{\lambda}_2 + ||x||^2 \frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_1 - \tilde{\lambda}_3}$$

If  $\theta_* = \pi/4$ , then  $\tilde{\lambda}_1 = \tilde{\lambda}_3 + ||x||^2$  and

$$\mu_* = \tilde{\lambda}_1$$

Finally, if  $\theta_* = \pi/2$ , then  $p(\theta_*) = 1$  and again

$$\mu_* = \tilde{\lambda}_1$$

Summarizing

$$\mu_* = \begin{cases} \tilde{\lambda}_1, & \tilde{\lambda}_1 \leq \tilde{\lambda}_3 + ||x||^2 \\ \frac{\tilde{\lambda}_1(\tilde{\lambda}_2 + ||x||^2) - \tilde{\lambda}_2(\tilde{\lambda}_3 + ||x||^2)}{\tilde{\lambda}_1 - \tilde{\lambda}_3}, & \tilde{\lambda}_1 > \tilde{\lambda}_3 + ||x||^2 \end{cases}$$

Now consider  $\mu_{**}$ . Observe that  $\cos \theta_{**} = \lim_{x_1 \rightarrow 0} \cos \theta = 0$ . So  $\theta_{**} = \pi/2$  and

$$r(\theta_{**}) = \cos^2(\pi/2 - \sigma(\theta_{**})\varphi_{\text{gap}}) = \sin^2 \varphi_{\text{gap}}$$

Thus

$$\begin{aligned} \mu_{**} &= \tilde{\lambda}_2 + ||x||^2 - ||x||^2 \sin^2 \varphi_{\text{gap}} = \tilde{\lambda}_2 + ||x||^2 - ||x||^2 \frac{\tilde{\lambda}_2 - \tilde{\lambda}_3}{\tilde{\lambda}_1 - \tilde{\lambda}_3} \\ &= \tilde{\lambda}_2 + ||x||^2 \frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_1 - \tilde{\lambda}_3} \end{aligned}$$

Next we see that  $d_1 = \tilde{\lambda}_1$  and  $d_2 = \tilde{\lambda}_2 + ||x||^2$ . Finally, one can check that

$$\min \{d_1, d_2, d_3\} = \tilde{\lambda}_1 \quad \text{for} \quad \tilde{\lambda}_1 \leq \tilde{\lambda}_3 + ||x||^2$$

and

$$\min \{d_1, d_2, d_3\} = \mu_* = \mu_{**} \quad \text{for } \tilde{\lambda}_1 > \tilde{\lambda}_3 + \|x\|^2$$

so

$$D_1(\rho_X) = \begin{cases} \tilde{\lambda}_1, & \tilde{\lambda}_1 \leq \tilde{\lambda}_3 + \|x\|^2 \\ \frac{\tilde{\lambda}_1(\tilde{\lambda}_2 + \|x\|^2) - \tilde{\lambda}_2(\tilde{\lambda}_3 + \|x\|^2)}{\tilde{\lambda}_1 - \tilde{\lambda}_3}, & \tilde{\lambda}_1 > \tilde{\lambda}_3 + \|x\|^2 \end{cases}$$

and this formula is in the full accordance with the results presented in [10].

### 7.5 The class containing quantum-classical states

Now we apply our results to the class of states with arbitrary Bloch vector  $x$  and correlation matrix having only one nonzero singular value. Such class, in particular, contains quantum-classical states [10]. We can always assume that

$$K = \begin{pmatrix} \kappa & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad x = \begin{pmatrix} x_1 \\ 0 \\ x_3 \end{pmatrix}$$

One can check that possible critical points lay on the big circle  $v_2 = 0$  or are given by  $(0, \pm 1.0)$ . By a direct inspection one gets that the minimal value can be achieved only on the circle  $v_2 = 0$ . So we are left with one-dimensional minimization problem. This can be done by a direct analysis (see [10]), but we apply our general result. To find value of  $D_1(\rho)$  we need only  $\mu_*$  and  $\mu_{**}$  which take the form

$$\mu_* = \kappa^2 (1 - p(\theta_*)), \quad \mu_{**} = \|x\|^2 (1 - r(\theta_{**}))$$

with  $\theta_* \in (\varphi_{\text{gap}}, \varphi_{\text{gap}})$  and  $\theta_{**} \in (-\pi/2, -\varphi_{\text{gap}}) \cup (\varphi_{\text{gap}}, \pi/2)$ . After a direct but quite lengthy computations one finds that the absolute minimum is given by  $\mu_*$  and the value of discord reads

$$D_1(\rho) = \frac{|\kappa| |x_3|}{\sqrt{(|\kappa| + |x_1|)^2 + x_3^2}}$$

Notice that this formula is in a full agreement with the result obtained in [10].

### 7.6 Beyond the X-states

Consider the following two-parameter family of states

$$\rho_{\gamma,a} = \frac{1}{4} \begin{pmatrix} 1 + a(1 + w_2) & -iaz & -iaz & a(2 - w_1) \\ ia z & 1 + a(1 - w_2) & a(2 + w_1) & ia z \\ ia z & a(2 + w_1) & 1 - a(1 + w_2) & ia z \\ a(2 - w_1) & -iaz & -iaz & 1 - a(1 - w_2) \end{pmatrix} \tag{7.3}$$

where for  $\tilde{\gamma} = \sqrt{1 + 16\gamma^2}$  we define

$$\begin{aligned} w_1 &= \frac{\sqrt{7 - \tilde{\gamma}}(\tilde{\gamma} - 1) + \sqrt{7 + \tilde{\gamma}}(\tilde{\gamma} + 1)}{2\sqrt{2}\tilde{\gamma}} \\ w_2 &= \frac{\sqrt{7 - \tilde{\gamma}}(\tilde{\gamma} + 1) + \sqrt{7 + \tilde{\gamma}}(\tilde{\gamma} - 1)}{2\sqrt{2}\tilde{\gamma}} \\ z &= \frac{\sqrt{7 + \tilde{\gamma}} - \sqrt{7 - \tilde{\gamma}}}{\tilde{\gamma}} \sqrt{2}\gamma \end{aligned}$$

One can check that (7.3) defines a state if  $|\gamma| \leq \sqrt{3}$  and  $a$  is the function of  $\gamma$ , known only numerically. The corresponding correlation matrix and Bloch vector are as follows:

$$K = a \begin{pmatrix} 2 & 0 & 0 \\ 0 & w_1 & z \\ 0 & z & w_2 \end{pmatrix}, \quad x = \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix}$$

so the parameter  $a$  is equal to the norm  $\|x\|$  of the Bloch vector. Interesting property of the above correlation matrix is that

$$K K^T = \|x\|^2 \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 2\gamma \\ 0 & 2\gamma & 3 \end{pmatrix}$$

so the matrix  $L_-$  is simple

$$L_- = \|x\|^2 \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 2\gamma \\ 0 & 2\gamma & 2 \end{pmatrix} \tag{7.4}$$

and the corresponding ordered eigenvalues are given in the explicit way

$$\begin{aligned} \tilde{\lambda}_1 &= \|x\|^2 \left( 3 + \sqrt{1 + 4\gamma^2} \right), \quad \tilde{\lambda}_2 = 4 \|x\|^2, \\ \tilde{\lambda}_3 &= \|x\|^2 \left( 3 - \sqrt{1 + 4\gamma^2} \right) \end{aligned} \tag{7.5}$$

Since the spectrum of  $L_-$  is non-degenerate, to find the value of  $D_1(\rho_{\gamma,a})$ , we must apply Theorem 6.1. First, notice that the Bloch vector in the basis of eigenvectors of  $L_-$  reads

$$x = \|x\| \begin{pmatrix} \frac{2\gamma}{\sqrt{2(1+4\gamma^2 + \sqrt{1+4\gamma^2})}} \\ 0 \\ \frac{-2\gamma}{\sqrt{2(1+4\gamma^2 - \sqrt{1+4\gamma^2})}} \end{pmatrix}$$

Then

$$\cos \varphi_{\text{gap}} = \frac{\sqrt{2}|\gamma|}{\sqrt{1+4\gamma^2 + \sqrt{1+4\gamma^2}}}, \quad \sin \varphi_{\text{gap}} = \frac{\sqrt{2}|\gamma|}{\sqrt{1+4\gamma^2 - \sqrt{1+4\gamma^2}}}$$

Since  $N_{**} = \|x\|^2$

$$\cos \theta_{**} = \frac{|x_1|}{\|x\|} = \frac{\sqrt{2}|\gamma|}{\sqrt{1+4\gamma^2 + \sqrt{1+4\gamma^2}}}$$

and

$$\sin \theta_{**} = -\frac{x_3 \text{sign}(x_1)}{\|x\|} = \frac{\sqrt{2}|\gamma|}{\sqrt{1+4\gamma^2 - \sqrt{1+4\gamma^2}}}$$

So  $\theta_{**} \in (0, \pi/2)$  and  $\theta_{**} = \varphi_{\text{gap}}$ . It follows that  $r(\theta_{**}) = 1$  and

$$\mu_{**} = \tilde{\lambda}_2 + \|x\|^2 - \|x\|^2 = \tilde{\lambda}_2 = 4\|x\|^2$$

Next, since  $N_* = \|x\|^2 \sqrt{1+16\gamma^2}$ , we obtain that

$$p(\theta_*) = \cos^2(\theta_* - \varphi_{\text{gap}}) = \frac{1}{2} \left( 1 - \frac{1}{\sqrt{1+16\gamma^2}} \right) = \frac{1}{2} \left( 1 - \frac{\|x\|^2}{N_*} \right)$$

So applying (6.6) we obtain

$$\mu_* = \frac{1}{2} \left( 7\|x\|^2 + N_* \left( 1 - \left( 1 - \frac{\|x\|^2}{N_*} \right) \right) \right) = 4\|x\|^2 = \mu_{**}$$

On the other hand

$$d_1 = \tilde{\lambda}_1 + x_1^2 = \|x\|^2 \left( 3 + \sqrt{1 + 16\gamma^2} \right) + x_1^2 > 4 \|x\|^2$$

and

$$d_2 = \frac{1}{2} \left( \tilde{\lambda}_1 + \tilde{\lambda}_2 + \|x\|^2 + x_3^2 - (\tilde{\lambda}_1 - \tilde{\lambda}_2) \right) = \tilde{\lambda}_2 + x_3^2 > \tilde{\lambda}_2$$

So

$$\min \{d_1, d_2, d_3\} = \mu_* = \mu_{**} = 4 \|x\|^2$$

and

$$D_1(\rho_{\gamma a}) = 2 \|x\|^2$$

## 8 Summary

Let us now summarize the results reported in the article. First, we have obtained new compact and elegant formula for the trace norm of the disturbance  $S(\mathcal{M})$  of the general two-qubit state. We want to emphasize that to obtain this result we have used the qubit structure of subsystems in the crucial way. In the general qudit case we were able only to find simplified formula for the square of the modulus of disturbance and only for the special classes of states [4]. It seems that the computation of trace norm of  $S(\mathcal{M})$  in general case is a highly non-trivial or even not possible at all. Then, we have applied the formula for  $\|S(\mathcal{M})\|_1$  to compute the value of geometric discord in the situation when the minimization procedure is not needed at all or is straightforward. This is the case of the class of states with arbitrary Bloch vectors and the correlation matrix proportional to some orthogonal matrix in three dimensions, i.e.,  $K = t V_0$ . In particular, for such states with zero Bloch vectors,  $\|S(\mathcal{M})\|_1 = |t|$  and  $D_1(\rho) = |t|$ . The presence of nonzero Bloch vectors only slightly changes the trace norm, and the minimization can be done in elementary way. This again must be contrasted with the general qudit case, where the similar results are valid only for vanishing Bloch vectors and the classes of Werner and isotropic states [4]. As a first step toward the computation of  $D_1(\rho)$  in general case, we considered critical points of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$ . To solve this problem, we introduce the function  $\mathbf{g}$  defined on the unit sphere  $\mathbb{S}^2 \subset \mathbb{R}^3$  with values in  $\mathbb{R}^2$ . Any critical point of the mapping  $\mathcal{M} \rightarrow \|S(\mathcal{M})\|_1$  is a critical point of the function  $\mathbf{g}$ , and the properties of this function can be used to isolate singular and smooth critical points. It is remarkable that the information about critical points is encoded in the spectrum of the matrix  $L_- = K K^T - W_x$ . One of the most important results of our study says that when this spectrum is non-degenerate, the critical points are located on big circles in  $\mathbb{S}^2$ . It means that the problem of finding geometric discord reduces to minimization of the quadratic form restricted to big circles. The complete

solution of this problem is rather involved, and it simplifies significantly, when any degeneracy of the spectrum of  $L_-$  is present.

We apply Theorems 6.1 and 6.2 to the cases already discussed in the literature (Bell diagonal, X-shaped and quantum-classical states) as well as new examples beyond the class of X-states. It is also worth to emphasize that, in particular, cases, methods based on partial results can be more efficient than the direct application of the general result, which is explicitly shown by the discussions of MMM states in Sects. 5.4 and 7.2.

Having the complete answer for the two-qubit system we are able to estimate possible obstacles in finding general explicit formula for the trace-distance quantum discord for qudits. As we have already stressed, the geometry of the two-qubit quantum state space is exceptional and the set of geometrical tools which is at our disposal is very reach. Let us recall here the most effective one that any correlation matrix can be diagonalized by means of local transformations, due to the accordance of the dimensions of relevant spaces and groups, i.e.,  $SO(3) \simeq \text{Adj}(SU(2))$ . For the next higher level system of two-qudits  $d = 3$  we have that  $\text{Adj}(SU(3))$  is a small subgroup of  $SO(8)$ , too small to allow diagonalization of a generic two-qudit correlation matrix by means of local transformations. For higher-dimensional cases this effect only aggravates, which means that using local orbit of the set of diagonal correlation matrices we can cover only a part of the quantum state space. The solution of the minimization problem for some families of two-qudit states is given in our previous works [4,12].

The strict analytical general formulas characterizing quantum correlations valid for all or sufficiently wide class of quantum states of compound systems, in general, are not known and only selected cases are described in the literature. Such explicit knowledge would be of value that hardly can be overestimated, as it gives insight into the structure of the quantum states, but, on the other hand, due to the complexity of this space, computation of physically important measures of quantum correlations is so hard task. We hope that results obtained in the present paper will fill the gap in the knowledge on measures of quantum correlations of compound systems for the most fundamental physical system of two qubits.

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