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Trace norm quantum discord for two qubits: the complete solution revisited and applications

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Abstract We have significantly improved the previous analysis of Ługiewicz et al. (Quantum Inf Process 18:185, 2019) in terms of several key issues. By emphasizing geometric arguments, for the first time we give a mathematically complete proof of the principle of three large circles on the unit sphere. This principle is one of the key ingredients of the whole reasoning on which our results are based. In addition, due to the elimination of difficult to use auxiliary special functions that were introduced earlier, we present now simplified formulae for the one-sided trace norm discord of any state of two qubits. We give applications of the new result in study of the state space. In particular, we propose an alternative classification of states, distinguish between self-adhered states, and discuss the complete description of the new class of states.

1 Introduction

In the literature of the subject, there is no commonly accepted consensus that indicates unambiguously which quantity should be chosen as a leading notion proper to describe the measure of quantum correlations. However, there are some distinguished features having well-accepted physical origin [1]. In particular, the quantum correlations hidden in any compound system should not increase under a local Schroedinger evolution. This criterion, which may be called the 'local evolution test', can be effectively used to exclude some of the definitions proposed as a measure of quantum correlations. In particular, this expected property is not present when one introduces the so-called geometric discord via the distance given by the Hilbert–Schmidt norm [2,3]. As opposed to the aforementioned Hilbert–Schmidt discord, the one-sided discord defined by distance in the sense of the trace norm between any state under consideration and the set of all classical-quantum or quantum-classical states was proposed in [2] as an analytically simpler replacement for the entropic quantum discord, and simultaneously as a quantity which is still being a suitable candidate that might give a right quantum correlation measure. In that regard, the (one-sided) trace norm discord or its weaker variety called the measurement-induced trace norm discord seems definitely to be attractive objects of interest as they pass positively the local evolution test, and moreover they do obey all the fundamental rules that should be respected by any physical measure of quantum correlations [1]. Also the measurement-induced trace norm discord is connected with the negativity of entanglement and can be directly expressed by the so-called minimum entanglement potential [4].

Since quite long time, the question of how to compute values of almost any measure describing quantum correlations in composite systems has been considered as a hard problem to be solved, if this purpose is possible to achieve, at all [5]. Of particular note is the fact that apart from the geometric discord based on the Hilbert–Schmidt norm [6], which, as we have already noted, is non-physical, the analytical formulae for other types of quantum correlations measures, even in the simplest cases, like the bipartite system of qubits, were given in the literature to a very modest and really narrow scope [1,5]. What should be emphasized more is that the analytical formula for the trace norm discord published in [2] is given for the Bell diagonal states, only, and the technique used by authors to get this result has been based to a significant extent on numerical computations. Here, the choice itself of the numerical support indicates clearly that the raised issues for computability of quantum correlations are really non-trivial to be solved by means of purely analytical methods even in the simpler cases, as well. Notwithstanding, in the case of two qubits some breakthrough can be noticed with the advent of [7] and the following [8] where the mathematical procedures presented there provide in principle a complete solution to the problem of computability for the one-sided trace norm discord defined as in [2]. Two-qubit systems tend to be unique because of their exceptional attributes; for example, the notion of the one-sided trace norm discord does coincide with the measurement-induced one-sided trace norm discord. Nevertheless, it seems to be quite surprising that there is a strong limitation in access to this type of results as given in [7,8] even in slightly more complex systems than two qubits, and the apparent lack of analytical methods is still present in such cases. This limitation is emerging whenever one tries to generalize the analysis of [7] or [8] to bipartite systems with higher spins involved [9,10]. For instance, except for the analysis presented in [10] that

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can be simplified under some strong assumptions like this that correlations matrices of states give rise to Jordan automorphisms of the corresponding spin algebra which occurs for isotropic or Werner states [11,12], in a bit more general cases one still firmly concludes that analytical expressions even for the measurement-induced one-sided trace norm discord of higher spin systems seem to be beyond the reach of currently known mathematical techniques. Unexpectedly, all mathematical difficulties already occur for systems made of two qutrits instead of two qubits. Indeed, if one looks at the very description of a single qutrit (i.e. a system with a spin equal to 1 or equivalently called 'three-level system'), then one will notice that it is much more complex than for a single qubit, and in particular the geometry of its state space has been only fragmentarily understood [13]. In point of fact, the main cause of the obstacles encountered may be seen in the circumstances that can be explained in the following way. Namely, the symmetry group for a qubit is given simply by the group $SU(2)$ that is the covering group of the rotation group $SO(3)$. In the case of a single qutrit, one uses $SU(3)$ as a symmetry group that is, in turn, the covering group of $AdSU(3)$. The latter group is merely a subgroup contained in the rotation group $SO(8)$. But above all else, the way in which $AdSU(3)$ subgroup is immersed in $SO(8)$ group is extremely peculiar and this sets all attempts of mathematical description at a very high level of complexity. The exact same mathematical issue is reflected in a similar situation if one deals with entanglement of mixed states. In that case, the structure of the cone formed by positive mappings for any algebra carrying a spin higher than $\frac{1}{2}$ remains not recognized enough [14]. It is extraordinarily difficult to detect new extremal positive mappings even for the spin one algebra [15,16] and examples of such mappings are indeed connected with a problem posed by Hilbert who himself failed to give any practical construction of a non-negative quaternary quartic form that is not a sum of squares of polynomials [17]. The lack in description of positive mappings causes that it is problematic to find so-called witnesses of entanglement [18] or to disprove their existence for a given state. Admittedly, the interest in a search for mild correlations described by discord and the vast number of recipes telling how to define it could be seen as a kind of a pragmatic response to the mathematical and physical difficulties appearing when dealing with the mixed states being entangled [1]. However, it turns out that higher spin systems in both regards: the entanglement and discord, incredibly are always much less controlled by the use of analytic methods.

On the other hand, it is well known that the quantum correlations, even the mild ones described by discord, play a significant role in an appearance of the positivity or complete positivity violation for dynamical maps [19,20]. This mathematical phenomenon fits to give an alternative new way for the description of the correlations contained in quantum systems as it manifests itself in a blurring of obvious boundaries between the system and its environment during the process of evolution of the system over time. More generally, the need to know explicit analytical formulas describing quantum correlations contained in states evolving over time seems to be important when trying to gain better insight into the behavior of quantum open systems, or even these simplest ones composed of several qubits. Again there is no analytical method proposed in this area of research, at all (see also for instance [21,22] where some exemplary numerical results are presented). Nowadays, the use of quantum correlations, the one that is probably the most desirable, is related to the implementation of quantum computing processes that can bring significant progress in accelerating the operation of future computers [23–26].

Below in our paper, we consider a bipartite system of two qubits, only, and we use the word 'discord' to name the one-sided discord related to the trace norm. In the previous article [8], the computability question of the discord has basically been completely answered, but the elaborated formulas refer to certain auxiliary special functions that make any use of the result obtained in [8] very hard or even impossible. In the present publication, we aim at a simplification of the final formulae for the discord to make them more convenient in use. Regrettably, despite all the efforts made to refine these formulas, the ultimate result is still quite complex if it is allowed to consider the most general cases. It must be so, as the sets of classical-quantum or quantum-classical states have got an elaborate structure and the geometry used is determined by the trace norm—very natural to study the space of states but rather much less intuitive and not directly manageable as, e.g., the Euclidean geometry provided by the Hilbert–Schmidt norm. Nevertheless, the main result of the present paper is a step to overcome these obstacles and furthermore it can be applied successfully to get new estimates for values of the discord or to uncover some new classes of states that have not been present in a common circulation of the scientists community, up to now. Indeed, we note that the mixed states most popular in use are the so-called X-states, as well as, the results given in [7] are, in principle, restricted to a class of states locally equivalent to them. Moreover, to our best knowledge, no one went essentially beyond X-states except an example given by the authors of [8]. Undeniably, the set of all states for two qubits is not sufficiently well understood with a vague geometrical interpretation. Hence it is still very interesting to gain new information about it. In our current article, we select and give a complete classifications of a new class of states that reveal some geometrical interpretation of the underlying minimizing procedure: the unit vector given by the direction of a Bloch vector designates the value of the discord (see (54) below). More generally, our analysis suggests a new classification in the set of all states of two qubits that can be used to provide a further detailed description for the whole space of states. At last, we mention our main motivation that guided us to undertake this intricate research: having established the full mathematical formula for the trace norm discord, what is indeed an exceptional circumstance as for measures of quantum correlations, one can next study the discord itself, its particular properties in full and consequently deepen the research on quantum correlations and their dynamics in complex or open systems. Undoubtedly, the knowledge about the trace norm discord is still limited by the fact that no one has got any reasonable control of its values in general. The current paper presents a part of a broader mathematical analysis needed to reach these objectives and therefore to clarify the role of the trace norm discord.

The organization of the paper is as follows. After Preliminaries, in the third section we recall briefly the necessary results obtained in [8] and then we present for the first time a complete mathematical argumentation leading to a rigorous proof of the fundamental thesis proposed in [8] and referred here as the principle of three large circles on the unit sphere. The fourth section is devoted to the formulation and the proof of our main result. In the fifth section, we show exemplary how the new results can be used to study the space of states for two qubits.

2 Preliminaries

In this section, we recall basic definitions and notations used in the paper. Let $\mathcal{M}$ be the set of all square matrices 2×2 with complex entries. $\mathsf{Tr}A$ means the trace of the matrix A. Let $\mathcal{M}_0$ be a subspace of $\mathcal{M}$ constituted by all traceless matrices from $\mathcal{M}$: $A \in \mathcal{M}_0$ iff $\mathsf{Tr}A = 0$. The standard Pauli matrices σ_k, $k = 1, 2, 3$ form a linear basis for $\mathcal{M}_0$. The general Hermitian matrix from $\mathcal{M}_0$ can be written as $\langle \mathsf{m}, \sigma\rangle = m_1\sigma_1 + m_2\sigma_2 + m_3\sigma_3$ with $\mathsf{m} = (m_1, m_2, m_3) \in \mathbb{R}^3$ and moreover $\mathbf{1}$ is the unit matrix 2×2. Below we use A^T—the transpose of A, and A^*—the Hermitian conjugation of A. For any 3×3 matrix I we consider the adjunct matrix $\mathsf{adj}I$ satisfying $I\,\mathsf{adj}I = \mathsf{det}I \cdot \mathbf{1}_3$ where $\mathbf{1}_3$ is the unit matrix 3×3. Any state $\varrho \in \mathbb{S}$ for the system of two qubits can be expressed in the unique way

$$\varrho = \frac{1}{4}\left[\mathbf{1} \otimes \mathbf{1} + \langle \mathsf{x}, \sigma\rangle \otimes \mathbf{1} + \mathbf{1} \otimes \langle \mathsf{y}, \sigma\rangle + \sum_{k,l=1}^{3} I_{kl}\sigma_k \otimes \sigma_l\right] \tag{1}$$

where $\mathsf{x} = \mathsf{Tr}\,(\varrho\sigma \otimes \mathbf{1})$, $\mathsf{y} = \mathsf{Tr}\,(\varrho\mathbf{1} \otimes \sigma)$ are some vectors $\mathsf{x}, \mathsf{y} \in \mathbb{R}^3$ that one calls the left and right Bloch vectors, correspondingly. The correlation matrix I is given by

$$I_{kl} = \mathsf{Tr}\,(\varrho\sigma_k \otimes \sigma_l) \qquad \text{for } k, l = 1, 2, 3$$

We equip the space $\mathbb{S}$ with the distance function given by the trace norm defined for any matrix A by $\|A\|_1 = \mathsf{Tr}\sqrt{A^*A}$. As a matter of fact $\varrho \in \mathbb{S}$ iff $\varrho \geq 0$ and moreover $\mathsf{Tr}\varrho = \|\varrho\|_1 = 1$. Let a pair $\{P_1, P_2\} \subset \mathcal{M}$ be called a complete pair of projectors if P_1, P_2 are any two orthogonal projectors such that $P_1 + P_2 = \mathbf{1}$, $P_1P_2 = \mathbf{0}$. The state $\rho \in \mathbb{S}$ is *classical-quantum* iff for some complete pair of projectors $\{P_1, P_2\}$ and some qubit states ρ_1 and ρ_2 there is $\rho = p_1P_1 \otimes \rho_1 + p_2P_2 \otimes \rho_2$ with non-negative numbers p_1, p_2 such that $p_1 + p_2 = 1$. The set of all classical-quantum states is denoted by $\mathbb{S}_{cq}$. Exchanging the position of projectors in the tensor product above we get the *quantum-classical* states $\mathbb{S}_{qc}$. The *left-side discord* of ϱ is defined by

$$D(\varrho) = \min\left\{\|\varrho - \rho\|_1 : \quad \rho \in \mathbb{S}_{cq}\right\} \tag{2}$$

The right-side discord is defined in the similar way if we use $\mathbb{S}_{qc}$ instead of $\mathbb{S}_{cq}$. All the results below are formulated for the left-side discord $D(\varrho)$, but one can easily pass to the right-side discord. If it matters we use the notation $D_L(\varrho)$ and $D_R(\varrho)$ to write the left-side or right-side discord, correspondingly. The main auxiliary objects are: the projectors P_{x} and P_{y} not normalized, defined as $P_{\mathsf{x}}\mathsf{v} = \langle \mathsf{x}, \mathsf{v}\rangle\mathsf{x}$. If the norm $\|\mathsf{x}\| = 1$, then P_{x} is an orthogonal projector. Moreover a crucial role is played by the following operators [8]:

$$L = II^T - P_{\mathsf{x}} \qquad \text{and} \qquad R = I^TI - P_{\mathsf{y}} \tag{3}$$

The oparator L is used when one considers the left-side discord $D_L(\varrho)$ and the operator R for the right-side discord $D_R(\varrho)$. Let P be a projector defined on the full matrix algebra:

$$\mathsf{P}(A) = \sum_{k=1,2} P_kAP_k \quad \text{for all } A \in \mathcal{M}$$

where $\{P_1, P_2\}$ is a complete pair of projectors. Let notice that $\mathsf{P}\mathcal{M}_0 \subset \mathcal{M}_0$ and hence the restriction $\mathsf{P}\restriction_{\mathcal{M}_0}$ makes sense and determines in an unique way an orthogonal projector P_{v} for some vector $\mathsf{v} \in \mathbb{R}^3$, $\|\mathsf{v}\| = 1$. Let $M_{\mathsf{v}} = \mathbf{1}_3 - P_{\mathsf{v}}$ then M_{v} is an orthogonal projector in $\mathbb{R}^3$ such that $\mathsf{Tr}M_{\mathsf{v}} = 2$. Let $\varPi_2$ be the set of all orthogonal projectors M in $\mathbb{R}^3$ such that $\mathsf{Tr}M = 2$. For any chosen and fixed state ϱ, one can consider the function [8]

$$\mu(M) = \|\varrho - \mathsf{P} \otimes \mathrm{id}_{\mathcal{M}}(\varrho)\|_1 \quad \text{for all } M \in \varPi_2 \tag{4}$$

then the left-side discord

$$D(\varrho) = \min\{\mu(M) : \quad M \in \varPi_2\} \tag{5}$$

The proof of (5) can be found in [4] and corresponds to the known statement that the measurement-induced discord is equivalent to the discord for the system of two qubits.

3 The principle of the three large circles on S^2

The minimizing procedure that should be done to get the value $D(\varrho)$ given by (5) is quite complex and very far to be intuitive. The remarkable key step to achieve it is the introduction of the operator L or R as defined in (3). It has been observed in [8] that if L (or R) has got a degenerate spectrum, then the formula for $D(\varrho)$ is given in a simple way. But if L (R, correspondingly) has got a non-degenerate spectrum, then the situation gets much more complex. In any case, the spectra of the operators L or R play a significant role in determining $D_L(\varrho)$ or $D_R(\varrho)$. Let $\tilde{\lambda}_k$, $k = 1, 2, 3$ be the set of eigenvalues of L, then in the case of a non-degenerate spectrum we introduce the order in the set of eigenvalues and at the same time in the set of eigenvectors by setting: $\tilde{\lambda}_1 > \tilde{\lambda}_2 > \tilde{\lambda}_3$ where $L\mathsf{w}_k = \tilde{\lambda}_k \mathsf{w}_k$ and $\mathsf{w}_1, \mathsf{w}_2, \mathsf{w}_3$ are the corresponding normalized eigenvectors of the operator L. We introduce the coefficients that describe the degree of a deviation from a degenerate spectrum: $\sqrt{a} = \tilde{\lambda}_1 - \tilde{\lambda}_2$, $\sqrt{b} = \tilde{\lambda}_2 - \tilde{\lambda}_3$. It is convenient to consider $\sqrt{c} = \sqrt{a} + \sqrt{b}$, as well. Let S^2 is the unit sphere in the Euclidean space $\mathbb{R}^3$. *The principle of the three large circles on* S^2:

The value of $D(\varrho)$ is assumed for such $M_* \in \Pi_2$ that the direction $\mathsf{v}_* \in \mathsf{S}^2$ defined by $P_{\mathsf{v}_*} = \mathbf{1}_3 - M_*$ does satisfy

$$v_1 v_2 v_3 = 0 \quad \text{where} \quad \mathsf{v}_* = v_1 \mathsf{w}_1 + v_2 \mathsf{w}_2 + v_3 \mathsf{w}_3$$

This principle is a heart of the analysis and is a crucial ingredient of the Theorem 4.1 that provides us with the general formula for the discord $D(\varrho)$ with L possessing a non-degenerate spectrum. A rigorous proof of this principle is rather a hard part of the whole reasoning. Therefore, we present below a new approach based on geometrical arguments to get a proof of this principle in a relatively simpler way compared to algebraic approach suggested in [8].

Theorem 3.1 *Let L have got a non-degenerate spectrum, then the principle of the three large circles on the unit sphere* S^2 *holds true.*

Let d be a function

$$2d = \omega + \sqrt{\omega^2 + 4\sqrt{ab}v_2^2} \qquad \text{for all } \mathsf{v} \in \mathsf{S}^2 \tag{6}$$

where $\omega = \sqrt{a} - \sqrt{c}v_1^2 - \sqrt{b}v_2^2$. We precede the proof of Theorem 3.1 by the lemma below

Lemma 3.1 *If the operator L has got a non-degenerate spectrum, then all critical points of the function d satisfy* $v_1 v_2 v_3 = 0$ *and moreover*

$$d = \begin{cases} \sqrt{a} & \textit{for} \quad v_1 = 0 \\ \left.\begin{matrix} \sqrt{a} - \sqrt{c}v_1^2 & \textit{for} \quad v_1^2 \in [0, \frac{\sqrt{a}}{\sqrt{c}}) \\ 0 & \textit{for} \quad v_1^2 \in [\frac{\sqrt{a}}{\sqrt{c}}, 1] \end{matrix}\right\} & \textit{for} \quad v_2 = 0 \\ \sqrt{a}v_2^2 & \textit{for} \quad v_3 = 0 \end{cases} \tag{7}$$

The lemma above suggests that the main idea of the proof of Theorem 3.1 is to show that the following perturbation of the function d

$$\tilde{\mu} = d - \langle \mathsf{x}, \mathsf{v} \rangle^2 \tag{8}$$

does not change the localization of its critical points in an essential way. That means: the minimum of $\tilde{\mu}$ is assumed in the set constituted by the same large circles of S^2 as in the case of the unperturbed function d. The relation between the auxiliary function $\tilde{\mu}$ and μ defined by (4) is given by the equation [8]

$$\mu = \tilde{\mu} + \tilde{\lambda}_2 + \|\mathsf{x}\|^2 \tag{9}$$

The Proof of the Theorem 3.1 We consider the functions $\tilde{\mu}$ and d as functions defined on the unit disk $\mathsf{D} = \{(v_1, v_2) \in \mathbb{R}^2 : \ v_1^2 + v_2^2 \le 1\}$.

This can be easily done as $\tilde{\mu}(-\mathsf{v}) = \tilde{\mu}(\mathsf{v})$, so it is enough to consider points v with $v_3 \ge 0$ and then each such point $\mathsf{v} = (v_1, v_2, v_3) \in \mathsf{S}^2$ has got the unique representation in D via the orthogonal projection of coordinates $\pi : (v_1, v_2, v_3) \to (v_1, v_2)$. Using the symmetries of the function d under the action of reflections: $d(\varepsilon_1 v_1, \varepsilon_2 v_2) = d(v_1, v_2)$ for any real $\varepsilon_1, \varepsilon_2$ with $\varepsilon_1^2 = \varepsilon_2^2 = 1$ and again using (8), one can show that, without any loss of generality, the analysis can be restricted to the case where $x_1, x_2, x_3 \ge 0$ and the region $\mathsf{D}_+ \subset \mathsf{D}$ determined by the condition $v_1, v_2 \ge 0$. Indeed, the reflection $\mathsf{x} \to -\mathsf{x}$ does not change $\tilde{\mu}$ and the minimum can be assumed in that region of the disk D where lies the orthogonal projection $\pi(\mathsf{x})$. Then using the reflections one can pass from x to x' where the projection of the last vector $\pi(\mathsf{x}')$ lies in D_+. This process does not change the function d. Therefore, to prove our theorem it is enough to show that the minimum of $\tilde{\mu}$ can not be assumed in the interior intD_+ that is given by all elements of D such that $v_1, v_2 > 0$ and $v_1^2 + v_2^2 < 1$. To this end, we consider two auxiliary vector fields ∂_H and ∂_H^* in the region intD_+ defined in the way described below. Let us fix any $\lambda \in (0, \sqrt{a})$, then for any point $(v_1, v_2) \in$intD_+ such that

$$\frac{\sqrt{c}}{\sqrt{a} - \lambda} v_1^2 - \frac{\sqrt{b}}{\lambda} v_2^2 = 1 \tag{10}$$

we define

$$\partial_H \Big|_{(v_1, v_2)} = \frac{\sqrt{b}}{\lambda} v_2 \frac{\partial}{\partial v_1}\Big|_{(v_1, v_2)} + \frac{\sqrt{c}}{\sqrt{a} - \lambda} v_1 \frac{\partial}{\partial v_2}\Big|_{(v_1, v_2)}$$

We note that the curves (10) for different values of λ do not intersect each other and all the curves do cover the open region $\mathrm{int}\mathsf{D}_+$ when varying $\lambda \in (0, \sqrt{a})$. In our analysis below, we need the second field that reads

$$\partial^*_H\Big|_{(v_1,v_2)} = (x_2 v_3 - x_3 v_2)\frac{\partial}{\partial v_1}\Big|_{(v_1,v_2)} + (x_3 v_1 - x_1 v_3)\frac{\partial}{\partial v_2}\Big|_{(v_1,v_2)}$$

for all $(v_1, v_2) \in \mathrm{int}\mathsf{D}_+$. We notice that these fields are horizontal, i.e.:

$$\partial_H d = 0 \quad \text{and} \quad \partial^*_H \langle \mathsf{x}, \mathsf{v}\rangle^2 = 0 \qquad \text{in the region } \mathrm{int}\mathsf{D}_+ \tag{11}$$

Hence the critical points $(u_1, u_2) \in \mathrm{int}\mathsf{D}_+$ of the function $\tilde{\mu}$ satisfy two additional conditions

$$\partial^*_H\big|_{(u_1,u_2)} d = 0 \quad \text{and} \quad \partial_H\big|_{(u_1,u_2)} \langle \mathsf{x}, \mathsf{v}\rangle^2 = 0 \tag{12}$$

The equations (12) give

$$\lambda\sqrt{c}(x_2u_3 - x_3u_2)u_1 - \sqrt{b}(2\sqrt{a} - \lambda)(x_3u_1 - x_1u_3)u_2 = 0 \tag{13}$$

and

$$\lambda(\sqrt{a}x_3u_1u_2 + \sqrt{b}x_1u_2u_3 - \sqrt{c}x_2u_3u_1) + \sqrt{ab}(x_3u_1 - x_1u_3)u_2 = 0 \tag{14}$$

If we admit that $x_3 = 0$, then the left-hand side of (14) is negative and we arrive at the contradiction. Therefore, we assume below that $x_3 > 0$. We add (13) and (14) together and obtain the first equation written below

$$\begin{aligned} x_1u_3 - x_3u_1 &= 0 \\ x_2u_3 - x_3u_2 &= 0 \end{aligned} \tag{15}$$

To get the second equation above, we insert the first one to (13). The condition (15) implies that $x_2 > 0$, $x_1 > 0$ and moreover $x_2u_1 - x_1u_2 = 0$. Let $\mathsf{u}_* = \mathsf{x}/\|\mathsf{x}\|$. Note that the field ∂^*_H is singular at $\pi(\mathsf{u}_*)$, and the analysis for this point should be supplemented by considering a derivative in a non-parallel direction to $\partial_H|_{\pi(\mathsf{u}_*)}$. By direct calculations

$$\frac{\partial}{\partial v_1}\Big|_{\pi(\mathsf{u}_*)} \tilde{\mu} = 0 \quad \Rightarrow \quad d(\pi(\mathsf{u}_*)) = 0$$

This can happen only when $u_2 = 0$, but this is impossible as (u_1, u_2) $\in\mathrm{int}\mathsf{D}_+$ by the assumption made. Consequently, we arrived at a contradiction and the proof is finished. □

To complete the discussion in this section, we recall the result obtained in [8] for the case when the operator L has got any degeneracy in its spectrum. It is worthy to note that in this case the basis of eigenvectors of L plays a crucial role but to a narrowed extent governed by a possible partial non-degeneracy.

Theorem 3.2 *Let L have got any degenarate eigenvalue then the discord $D(\varrho)$ is given by*

$$D(\varrho)^2 = \frac{1}{2}\left\{\tilde{\lambda}_1 + \tilde{\lambda}_2 + \|\mathsf{x}\|^2 - \sqrt{\left[\tilde{\lambda}_1 - \tilde{\lambda}_2 + \|\mathsf{x}\|^2\right]^2 - 4(\tilde{\lambda}_1 - \tilde{\lambda}_2)\left[\|x\|^2 - x_1^2\right]}\right\} \tag{16}$$

The similar constructions and an analogical principle of the three large circles can be considered for the operator R, but we omit the detailed formulation due to the direct similarity to the case of L.

4 Analytical formulae for $D(\varrho)$: the case of L (or R) with a non-degenerate spectrum

Below we always assume that the spectrum of the operator L is non-degenerate. Having Theorem 3.1, one can find the minimum of μ by a restriction of this function to the domain given by the three large circles of S^2 as described in the previous section. It has been done in [8]. The final expression describing the discord $D(\varrho)$ has got a complex structure. In this section, we present the analysis that makes possible the better understanding of the formula for $D(\varrho)$ and consequently we are led to the partial analytical expressions in a more concise form than those ones given in the paper [8]. The present discussion we begin with a recalling some of definitions and notions introduced in [8]. Let φ_{gap} be the gap angle from $(0, \frac{\pi}{2})$ determined by

$$\cos\varphi_{\text{gap}} = \sqrt{\frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_1 - \tilde{\lambda}_3}} \tag{17}$$

Let $\sigma : [-\pi, \pi] \longrightarrow \{-1, 1\}$ be a function such that $\sigma(\Theta) = 1$ for all $\Theta \in (-\pi, -\frac{\pi}{2}) \cup (0, \frac{\pi}{2})$ and $\sigma(\Theta) = -1$ for any $\Theta \in (-\frac{\pi}{2}, 0) \cup (\frac{\pi}{2}, \pi)$. Next we consider the open set

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

The first special function reads

$$p_L(\Theta) = \begin{cases} 1 \quad \text{for} \quad \Theta \in \mathsf{O}_{\text{gap}} \\ \cos^2\left(\Theta - \sigma(\Theta)\varphi_{\text{gap}}\right) \quad \text{for} \quad \Theta \in [-\pi, \pi]\backslash\mathsf{O}_{\text{gap}} \end{cases} \tag{18}$$

where the subscript L means that this function is related to the operator L. The second function is as follows:

$$r_L(\Theta) = \begin{cases} \cos^2\left(\Theta - \sigma(\Theta)\varphi_{\text{gap}}\right) \quad \text{for} \quad \Theta \in \mathsf{O}_{\text{gap}} \\ 1 \quad \text{for} \quad \Theta \in [-\pi, \pi]\backslash\mathsf{O}_{\text{gap}} \end{cases} \tag{19}$$

Using these functions, one introduces

$$\mu_* = \frac{1}{2}\left\{\tilde{\lambda}_1 + \tilde{\lambda}_3 + \|\mathsf{x}\|^2 + x_2^2 + N_*(1 - 2p_L(\Theta_*))\right\} \tag{20}$$

where for $x_1x_3 \neq 0$ the angle Θ_* satisfies

$$\cos\Theta_* = \frac{\sqrt{2}|x_1x_3|}{\sqrt{N_*(N_* - \tilde{\lambda}_1 + \tilde{\lambda}_3 - x_1^2 + x_3^2)}} \tag{21}$$

$$\sin\Theta_* = -\frac{\sqrt{2}x_1x_3}{\sqrt{N_*(N_* + \tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 - x_3^2)}} \tag{22}$$

with

$$N_* = \sqrt{\left(\tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 - x_3^2\right)^2 + 4x_1^2x_3^2} = \sqrt{\left(\tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 + x_3^2\right)^2 - 4\left(\tilde{\lambda}_1 - \tilde{\lambda}_3\right)x_3^2} \tag{23}$$

If $x_1x_3 = 0$, then we use (21) and (22) given for $x_1x_3 \neq 0$ and next we pass to one-sided limits, e.g.: $x_1x_3 \to 0^+$ or 0^-. It can happen that the left and right limit are not the same but have got the opposite sings. However, it makes no confusion as the function p_L gives the same result in such cases.

Let

$$\mu_{**} = \tilde{\lambda}_2 + \|\mathsf{x}\|^2 - (\|\mathsf{x}\|^2 - x_2^2)r_L(\Theta_{**}) \tag{24}$$

where

$$\cos\Theta_{**} = \frac{|x_1|}{\sqrt{\|\mathsf{x}\|^2 - x_2^2}} \tag{25}$$

$$\sin\Theta_{**} = -\frac{x_3\,\text{sign}(x_1)}{\sqrt{\|\mathsf{x}\|^2 - x_2^2}} \tag{26}$$

We use the same remark as above when $x_1x_3 = 0$ as the function r_L exhibits a similar property as p_L.

Next let us consider the matrix entries of II^T given in the ordered basis formed by eigenvectors of L:

$$\mathsf{j}_k = (II^T)_{kk}$$

Let $D^{(\pm)}$ be the new auxiliary matrix

$$\pm D_{kl}^{(\pm)} = \mathsf{j}_k - \mathsf{j}_l \pm \sqrt{(\mathsf{j}_k - \mathsf{j}_l)^2 + 4x_k^2x_l^2}$$

We note that in the expression above we take simultaneously on both sides exclusively the upper signs or bottom ones. In particular $D_{kl}^{(+)} \geq D_{kl}^{(-)} \geq 0$. The main result of the paper is presented in the following theorem

Theorem 4.1 *Let the spectrum of the operator L be non-degenerate. The expression describing the left-side discord $D(\varrho)$ is given by the square root of the minimum* $\min\{\mu_1, \mu_2, \mu_*, \mu_{**}\}$ *where the following four numbers are listed below:*

$$\mu_1 = \mathsf{j}_1 \tag{27}$$

$$\mu_2 = \mathsf{j}_1 - \frac{1}{2}D_{12}^{(+)} + x_3^2 = \mathsf{j}_2 - \frac{1}{2}D_{12}^{(-)} + x_3^2 \tag{28}$$

$$\mu_* = \begin{cases} \mathsf{j}_2 + (|x_3|\cos\varphi_{\text{gap}} - |x_1|\sin\varphi_{\text{gap}})^2 & \textit{for} \quad \frac{1}{2}D_{13}^{(+)}[\tan^2\varphi_{\text{gap}} - 1] \geq -(\mathsf{j}_1 - \mathsf{j}_3) \\ \mathsf{j}_1 - \frac{1}{2}D_{13}^{(+)} + x_2^2 & \textit{for} \quad \frac{1}{2}D_{13}^{(+)}[\tan^2\varphi_{\text{gap}} - 1] < -(\mathsf{j}_1 - \mathsf{j}_3) \end{cases} \tag{29}$$

and

$$\mu_{**} = \begin{cases} j_2 & \textit{for} \quad |x_3| \le |x_1| \tan\varphi_{\rm gap} \\ j_2 + (|x_3|\cos\varphi_{\rm gap} - |x_1|\sin\varphi_{\rm gap})^2 & \textit{for} \quad |x_3| > |x_1|\tan\varphi_{\rm gap} \end{cases} \tag{30}$$

All the objects above are given in the ordered basis formed from eigenvectors of L.

The proof of the Theorem 4.1 The proof of Theorem 4.1 is quite lengthy; hence, we have divided it into several parts. At the very beginning, we remark that the numbers μ_1, μ_2, μ_*, μ_{**} appearing in the statement above represent the minimal values one can get by the minimizing procedure of the function μ restricted separately to each of the three large circles on S^2 (see [8] for more details). According to the principle of the three large circles, the least number of them gives the square of the discord $D(\varrho)$. The values μ_1 and μ_2 are directly taken from [8], and they are already given in the simple form therefore we do not discuss them below. But the quantities μ_* and μ_{**} are the ones that need the further analysis as they are represented in the complex way defined by (20) and (24) above. In other words, it suffices to show that (29) and (30) hold true to complete the proof. □

The common expression used in the definition of both special functions p_L and r_L given in (18) and (19) can be written as:

$$\begin{aligned} \cos^2(\Theta - \sigma(\Theta)\varphi_{\rm gap}) &= [\cos(\Theta)\cos(\varphi_{\rm gap}) + \underbrace{\sigma(\Theta)}_{\mathrm{sign}(\Theta)} \sin(\Theta)\sin(\varphi_{\rm gap})]^2 \\ &= \cos^2\Theta\cos^2\varphi_{\rm gap} + \sin^2\Theta\sin^2\varphi_{\rm gap} + 2\mathrm{sign}\Theta\sin\Theta\cos\Theta\sin\varphi_{\rm gap}\cos\varphi_{\rm gap} \end{aligned} \tag{31}$$

where, without any loss of generality, one can assume that $\Theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. Moreover

$$\left[-\frac{\pi}{2}, \frac{\pi}{2}\right] \setminus O_{\rm gap} = [-\varphi_{\rm gap}, \varphi_{\rm gap}]$$

and

$$\left[-\frac{\pi}{2}, \frac{\pi}{2}\right] \cap O_{\rm gap} = \left[-\frac{\pi}{2}, -\varphi_{\rm gap}\right) \cup \left(\varphi_{\rm gap}, \frac{\pi}{2}\right]$$

We establish the value $p_L(\Theta_*)$ given by (18) where $\Theta_* \in [-\varphi_{\rm gap}, \varphi_{\rm gap}]$. According to (23), (21) and (17), the common denominator of all expressions standing on the r.h.s of (31) takes form:

$$\begin{aligned} &\left(\tilde\lambda_1 - \tilde\lambda_3\right) N_* \left(N_* - \tilde\lambda_1 + \tilde\lambda_3 - x_1^2 + x_3^2\right)\left(N_* + \tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2\right) \\ &= \left(\tilde\lambda_1 - \tilde\lambda_3\right) N_* \left(N_*^2 - \left(\tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2\right)^2\right) = 4x_1^2x_3^2\left(\tilde\lambda_1 - \tilde\lambda_3\right) N_* \end{aligned} \tag{32}$$

The numerator standing in the total expression on the r.h.s of (31) is more complex. The first two summands of the numerator are:

$$\begin{aligned} &\left(\tilde\lambda_1 - \tilde\lambda_2\right) 2x_1^2x_3^2 \left(N_* + \tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2\right) \\ &+ \left(\tilde\lambda_2 - \tilde\lambda_3\right) 2x_1^2x_3^2 \left(N_* - \tilde\lambda_1 + \tilde\lambda_3 - x_1^2 + x_3^2\right) \end{aligned} \tag{33}$$

and the last one reads

$$\begin{aligned} &2\sqrt{\tilde\lambda_1 - \tilde\lambda_2}\sqrt{\tilde\lambda_2 - \tilde\lambda_3}\sqrt{N_* - \tilde\lambda_1 + \tilde\lambda_3 - x_1^2 + x_3^2}\sqrt{N_* + \tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2} \\ &\times \mathrm{sign}\Theta_* \left(-\mathrm{sign}\left(x_1x_3\right)\right) 2x_1^2x_3^2 \end{aligned} \tag{34}$$

with the cross × meaning that the multiplication factor is moved to another line. We notice also that

$$-\,\mathrm{sign}(x_1x_3) = \mathrm{sign}(\sin\Theta_*) = \mathrm{sign}\Theta_* \tag{35}$$

where the last equality holds true since $\Theta_* \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. Hence (34) takes the form:

$$\begin{aligned} &4\sqrt{\tilde\lambda_1 - \tilde\lambda_2}\sqrt{\tilde\lambda_2 - \tilde\lambda_3}x_1^2x_2^2\sqrt{N_*^2 - \left(\tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2\right)^2} \\ &= 8\sqrt{\tilde\lambda_1 - \tilde\lambda_2}\sqrt{\tilde\lambda_2 - \tilde\lambda_3}x_1^2x_3^2|x_1x_3| \end{aligned} \tag{36}$$

The expression (33) we can write as:

$$\begin{aligned} 2x_1^2x_3^2 \Big[&\left(\tilde\lambda_1 - \tilde\lambda_2\right) N_* + \left(\tilde\lambda_2 - \tilde\lambda_3\right) N_* + \left(\tilde\lambda_1 - \tilde\lambda_2\right)\left(\tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2\right) + \\ &- \left(\tilde\lambda_2 - \tilde\lambda_3\right)\left(\tilde\lambda_1 - \tilde\lambda_3 + x_1^2 - x_3^2\right)\Big] \end{aligned}$$

or in the equivalent way:

$$2x_1^2x_3^2\left[\left(\tilde{\lambda}_1-\tilde{\lambda}_3\right)N_*+\left[\tilde{\lambda}_1-\tilde{\lambda}_2-\left(\tilde{\lambda}_2-\tilde{\lambda}_3\right)\right]\left(\tilde{\lambda}_1-\tilde{\lambda}_3+x_1^2-x_3^2\right)\right] \tag{37}$$

All terms from (32), (36) and (37) gathered together give the formula for $p_L(\Theta_*)$

$$p_L(\Theta_*)=\frac{1}{2}+\frac{1}{2N_*}\left(\tilde{\lambda}_1+\tilde{\lambda}_3-2\tilde{\lambda}_2\right)+\frac{1}{2N_*\left(\tilde{\lambda}_1-\tilde{\lambda}_3\right)}\left\{\ \dots\ \right\}$$

where the expression in the bracket $\{\dots\}$ has got the form:

$$\begin{aligned}&\left(\tilde{\lambda}_1-\tilde{\lambda}_2\right)x_1^2+\left(\tilde{\lambda}_2-\tilde{\lambda}_3\right)x_3^2+2\sqrt{\tilde{\lambda}_1-\tilde{\lambda}_2}\sqrt{\tilde{\lambda}_2-\tilde{\lambda}_3}|x_1x_3|+\\&-\left[\left(\tilde{\lambda}_1-\tilde{\lambda}_2\right)x_3^2+\left(\tilde{\lambda}_2-\tilde{\lambda}_3\right)x_1^2-2\sqrt{\tilde{\lambda}_1-\tilde{\lambda}_2}\sqrt{\tilde{\lambda}_2-\tilde{\lambda}_3}|x_1x_3|\right]\end{aligned}$$

or equivalently:

$$\left(|x_1|\sqrt{\tilde{\lambda}_1-\tilde{\lambda}_2}+|x_3|\sqrt{\tilde{\lambda}_2-\tilde{\lambda}_3}\right)^2-\left(|x_1|\sqrt{\tilde{\lambda}_2-\tilde{\lambda}_3}-|x_3|\sqrt{\tilde{\lambda}_1-\tilde{\lambda}_2}\right)^2$$

If one uses (17), then the function $p_L(\Theta_*)$ can be written:

$$\begin{aligned}p_L(\Theta_*)=\frac{1}{2}+\frac{1}{2N_*}&\Big\{\tilde{\lambda}_1+\tilde{\lambda}_3-2\tilde{\lambda}_2+\\&+\left[|x_1|\cos\varphi_{\text{gap}}+|x_3|\sin\varphi_{\text{gap}}\right]^2-\left[|x_1|\sin\varphi_{\text{gap}}-|x_3|\cos\varphi_{\text{gap}}\right]^2\Big\}\end{aligned} \tag{38}$$

The use of the formula above leads to

$$\begin{aligned}N_*\left(1-2p_L(\Theta_*)\right)=2\tilde{\lambda}_2-\tilde{\lambda}_1-\tilde{\lambda}_3+\left(|x_1|\sin\varphi_{\text{gap}}-|x_3|\cos\varphi_{\text{gap}}\right)^2+\\-\left(|x_1|\cos\varphi_{\text{gap}}+|x_3|\sin\varphi_{\text{gap}}\right)^2\end{aligned} \tag{39}$$

After all these transformations, we are ready now to prove the lemma below:

Lemma 4.1 *The following formula holds true*

$$\mu_*=\begin{cases}\tilde{\lambda}_2+x_2^2+\left(|x_1|\sin\varphi_{\text{gap}}-|x_3|\cos\varphi_{\text{gap}}\right)^2 & \textit{for}\quad \Theta_*\in\left[-\varphi_{\text{gap}},\varphi_{\text{gap}}\right]\\ \frac{1}{2}\left[\tilde{\lambda}_1+\tilde{\lambda}_3+\|\mathbf{x}\|^2+x_2^2-N_*\right] & \textit{for}\quad \Theta_*\in\left[-\frac{\pi}{2},-\varphi_{\text{gap}}\right)\cup\left(\varphi_{\text{gap}},\frac{\pi}{2}\right]\end{cases} \tag{40}$$

The proof of the lemma: If $\Theta_*\in\left[-\varphi_{\text{gap}},\varphi_{\text{gap}}\right]$ then using (39) and (20) we can write down the expression for μ_*

$$\begin{aligned}2\mu_*&=2\tilde{\lambda}_2+2x_2^2+|x_1|^2+|x_3|^2-\left(|x_1|\cos\varphi_{\text{gap}}+|x_3|\sin\varphi_{\text{gap}}\right)^2\\&\quad+\left(|x_1|\sin\varphi_{\text{gap}}-|x_3|\cos\varphi_{\text{gap}}\right)^2\end{aligned}$$

or equivalently

$$\begin{aligned}2\mu_*&=2\tilde{\lambda}_2+2x_2^2+|x_1|^2\left(1-\cos^2\varphi_{\text{gap}}\right)+|x_3|^2\left(1-\sin^2\varphi_{\text{gap}}\right)\\&\quad-2|x_1||x_3|\cos\varphi_{\text{gap}}\sin\varphi_{\text{gap}}+\left(|x_1|\sin\varphi_{\text{gap}}-|x_3|\cos\varphi_{\text{gap}}\right)^2\end{aligned}$$

and hence we get the upper part of (40). If $\Theta_*\in\left[-\frac{\pi}{2},-\varphi_{\text{gap}}\right)\cup\left(\varphi_{\text{gap}},\frac{\pi}{2}\right]$, then referring to (18) and making use of (20) we obtain that $1-2p_L(\Theta_*)=-1$ and the statement of the lemma follows.

The analysis presented above we repeat now for the quantity μ_{**}. We need to consider the function $r_L(\Theta_{**})$ defined by (19) with $\Theta_{**}\in\left[-\frac{\pi}{2},-\varphi_{\text{gap}}\right)\cup\left(\varphi_{\text{gap}},\frac{\pi}{2}\right]$. We go back to the expression (31) where according to (25) and (17) the common denominator of the expression standing on the right-hand side of (31) reads now:

$$\left(\tilde{\lambda}_1-\tilde{\lambda}_3\right)\left(\|\mathbf{x}\|^2-x_2^2\right)=\left(\tilde{\lambda}_1-\tilde{\lambda}_3\right)\left(x_1^2+x_3^2\right) \tag{41}$$

To get the numerator of (31), we do not need to make an additional complement since all expressions in (31) have got a common denominator given above by (41), so:

$$x_1^2\left(\tilde{\lambda}_1-\tilde{\lambda}_2\right)+x_3^2\left(\tilde{\lambda}_2-\tilde{\lambda}_3\right)+2x_3|x_1|(-\text{sign}x_1)\text{sign}(\Theta_{**})\sqrt{\tilde{\lambda}_1-\tilde{\lambda}_2}\sqrt{\tilde{\lambda}_2-\tilde{\lambda}_3}$$

where

$$\mathrm{sign}\Theta_{**} = \mathrm{sign}(\sin\Theta_{**}) = -\mathrm{sign}(x_3)\mathrm{sign}(x_1)$$

hence

$$x_3\mathrm{sign}(\Theta_{**})(-\mathrm{sign}x_1) = |x_3|\mathrm{sign}(\Theta_{**})(-\mathrm{sign}x_3)\mathrm{sign}x_1 = |x_3|$$

According to the reasoning above, the expression for the numerator takes its final form:

$$x_1^2\left(\tilde{\lambda}_1-\tilde{\lambda}_2\right)+x_3^2\left(\tilde{\lambda}_2-\tilde{\lambda}_3\right)+2|x_1||x_3|\sqrt{\tilde{\lambda}_1-\tilde{\lambda}_2}\sqrt{\tilde{\lambda}_2-\tilde{\lambda}_3} \tag{42}$$

Using (41) and (42), we get for $\Theta_{**} \in \left[-\frac{\pi}{2}, -\varphi_{\mathrm{gap}}\right) \cup \left(\varphi_{\mathrm{gap}}, \frac{\pi}{2}\right]$:

$$r_L(\Theta_{**}) = \frac{1}{x_1^2+x_3^2}\left(|x_1|\cos\varphi_{\mathrm{gap}}+|x_3|\sin\varphi_{\mathrm{gap}}\right)^2 \tag{43}$$

We are ready to show that □

Lemma 4.2 *The following formula holds true*

$$\mu_{**} = \begin{cases} \tilde{\lambda}_2 + x_2^2 + \left(|x_1|\sin\varphi_{\mathrm{gap}} - |x_3|\cos\varphi_{\mathrm{gap}}\right)^2 \\ \qquad\qquad \textit{for}\ \ \Theta_{**} \in \left[-\frac{\pi}{2}, -\varphi_{\mathrm{gap}}\right) \cup \left(\varphi_{\mathrm{gap}}, \frac{\pi}{2}\right] \\ \tilde{\lambda}_2 + x_2^2 \qquad\qquad \textit{for}\ \ \Theta_{**} \in \left[-\varphi_{\mathrm{gap}}, \varphi_{\mathrm{gap}}\right] \end{cases} \tag{44}$$

The proof of the lemma: If $\Theta_{**} \in \left[-\frac{\pi}{2}, -\varphi_{\mathrm{gap}}\right) \cup \left(\varphi_{\mathrm{gap}}, \frac{\pi}{2}\right]$, then making use of (43) and (24) we get:

$$\mu_{**} = \tilde{\lambda}_2 + \|\mathbf{x}\|^2 - \left(|x_1|\cos\varphi_{\mathrm{gap}}+|x_3|\sin\varphi_{\mathrm{gap}}\right)^2$$

We raise the expression standing in the bracket to the power two

$$\mu_{**} = \tilde{\lambda}_2 + x_1^2 + x_2^2 + x_3^2 - x_1^2\cos^2\varphi_{\mathrm{gap}} - x_3^2\sin^2\varphi_{\mathrm{gap}} - 2|x_1||x_3|\sin\varphi_{\mathrm{gap}}\cos\varphi_{\mathrm{gap}}$$

We group terms standing by x_1^2 and x_3^2, and next we use that the sum of squares of sine and cosine equals to one. We obtain:

$$\mu_{**} = \tilde{\lambda}_2 + x_2^2 + x_1^2\sin^2\varphi_{\mathrm{gap}} + x_3^2\cos^2\varphi_{\mathrm{gap}} - 2|x_1||x_3|\sin\varphi_{\mathrm{gap}}\cos\varphi_{\mathrm{gap}}$$

and finally we arrive at

$$\mu_{**} = \tilde{\lambda}_2 + x_2^2 + \left(|x_1|\sin\varphi_{\mathrm{gap}} - |x_3|\cos\varphi_{\mathrm{gap}}\right)^2$$

This ends first part of the proof. If $\Theta_{**} \in \left[-\varphi_{\mathrm{gap}}, \varphi_{\mathrm{gap}}\right]$, then according to (19) the formula (43) gives that the function r_L assumes the value 1. Once again referring to (24), we obtain:

$$\mu_{**} = \tilde{\lambda}_2 + \|\mathbf{x}\|^2 - \|\mathbf{x}\|^2 + x_2^2 = \tilde{\lambda}_2 + x_2^2$$

and this is the end of the proof. □

To finish the proof of Theorem 4.1, we need to eliminate the angles Θ_* and Θ_{**} from the statement of the Lemmas 4.1 and 4.2. Let the symbol $\Box \in \{<, >, \leq, \geq\}$, then the following relations hold true

$$\begin{aligned} |x_3| \ \Box\ |x_1|\tan\varphi_{\mathrm{gap}} \ &\Leftrightarrow\ |\Theta_{**}| \ \Box\ \varphi_{\mathrm{gap}} \\ N_*\cos 2\varphi_{\mathrm{gap}} \ \Box\ \tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 - x_3^2 \ &\Leftrightarrow\ |\Theta_*| \ \Box\ \varphi_{\mathrm{gap}} \end{aligned} \tag{45}$$

where we recall that $N_* = \sqrt{(\tilde{\lambda}_1 - \tilde{\lambda}_3 + x_1^2 - x_3^2)^2 + 4x_1^2x_3^2} = \frac{1}{2}\left(D_{13}^{(+)} + D_{13}^{(-)}\right)$.

The second condition (45) can be rewritten as

$$-(\mathrm{j}_1 - \mathrm{j}_3) \ \Box\ \frac{1}{2}D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] \ \Leftrightarrow\ |\Theta_*| \ \Box\ \varphi_{\mathrm{gap}} \tag{46}$$

or

$$D_{13}^{(-)} \ \Box\ D_{13}^{(+)}\tan^2\varphi_{\mathrm{gap}} \ \Leftrightarrow\ |\Theta_*| \ \Box\ \varphi_{\mathrm{gap}} \tag{47}$$

We shall use (45) in the form given by (46) or (47). As a result of these considerations, we arrive at statement of the Theorem 4.1 and we end up its proof. □

Theorem 4.1 given above presents clearly that the further analysis needed to deepen the understanding of the derived formulae is rather a very tedious work. One may also notice that despite the significant simplifications gained by the elimination of the special functions r_L, p_L given by (18), (19) and in particular the elimination of the unhandy angles Θ_*, Θ_{**} causing practical difficulties in straightforward usage of the previous formula for $D(\varrho)$ given in [8], the new stage we arrived now gives the final formula that has got still a quite elaborate form. In this regard, we note that this takes place because the set of classical-quantum states $\mathbb{S}_{cq}$ used as the reference states (or quantum-classical $\mathbb{S}_{qc}$, correspondingly) has got an unclear affine structure, as e.g. $\mathbb{S}_{cq}$ is not a convex set. Besides, the geometry provided by the trace norm increases the complications seen in the final result. One notices, therefore, any further improvements are just impossible to get as the subject of study does not allow for that. Finally, we remark that the additional obstacles are formed by the lack of a practical description of the space of all states ϱ by the parameters introduced by (1), i.e. in particular we do not know in a straightforward way when the quantities j_k, $k = 1, 2, 3$ and the coordinates x_k, $k = 1, 2, 3$ of the Bloch vector x lead to positive defined matrices given by (1).

However, in the face of all difficulties listed above, the Theorem 4.1 leads us consequently to distinguish the following classes of states according to the four possible choices in (45) as given below:

The Class I.: $|x_3| \le |x_1| \tan\varphi_{\mathrm{gap}}$ and $D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] \ge -2(\mathrm{j}_1 - \mathrm{j}_3)$

$$D(\varrho)^2 = \begin{cases} \min\{\mathrm{j}_1, \mathrm{j}_2\} & \text{for } -\frac{1}{2}D_{12}^{(+)} + x_3^2 \ge 0 \\ \mathrm{j}_2 & \text{for } -\frac{1}{2}D_{12}^{(+)} + x_3^2 < 0, \quad -\frac{1}{2}D_{12}^{(-)} + x_3^2 \ge 0 \\ \mathrm{j}_2 - \frac{1}{2}D_{12}^{(-)} + x_3^2 & \text{for } -\frac{1}{2}D_{12}^{(+)} + x_3^2 < 0, \quad -\frac{1}{2}D_{12}^{(-)} + x_3^2 < 0 \end{cases} \tag{48}$$

The Class II.: $|x_3| \le |x_1| \tan\varphi_{\mathrm{gap}}$ and $D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] < -2(\mathrm{j}_1 - \mathrm{j}_3)$

$$D(\varrho)^2 = \begin{cases} \min\{\mathrm{j}_1, \mathrm{j}_2\} & \text{for } -\frac{1}{2}D_{12}^{(-)} + x_3^2 \ge 0, \quad -\frac{1}{2}D_{13}^{(+)} + x_2^2 \ge 0 \\ \min\{\mathrm{j}_1 - \frac{1}{2}D_{13}^{(+)} + x_2^2, \mathrm{j}_2\} & \text{for } -\frac{1}{2}D_{12}^{(-)} + x_3^2 \ge 0, \quad -\frac{1}{2}D_{13}^{(+)} + x_2^2 < 0 \\ \mathrm{j}_1 - \frac{1}{2}D_{12}^{(+)} + x_3^2 & \text{for } -\frac{1}{2}D_{12}^{(-)} + x_3^2 < 0, \quad -\frac{1}{2}D_{13}^{(+)} + x_2^2 \ge 0 \\ \mathrm{j}_1 + \min\{-\frac{1}{2}D_{12}^{(-)} + x_3^2, -\frac{1}{2}D_{13}^{(+)} + x_2^2\} & \text{for } \\ \qquad -\frac{1}{2}D_{12}^{(-)} + x_3^2 < 0, \quad -\frac{1}{2}D_{13}^{(+)} + x_2^2 < 0 \end{cases} \tag{49}$$

The Class III.: $|x_3| > |x_1| \tan\varphi_{\mathrm{gap}}$ and $D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] \ge -2(\mathrm{j}_1 - \mathrm{j}_3)$

$$D(\varrho)^2 = \begin{cases} \min\{\mathrm{j}_1, \mathrm{j}_2 + (|x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}})^2\} & \text{for } -\frac{1}{2}D_{12}^{(+)} + x_3^2 \ge 0 \\ \mathrm{j}_2 + \min\{-\frac{1}{2}D_{12}^{(-)} + x_3^2, (|x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}})^2\} & \\ \qquad \text{for } -\frac{1}{2}D_{12}^{(+)} + x_3^2 < 0 \end{cases} \tag{50}$$

The Class IV.: $|x_3| > |x_1| \tan\varphi_{\mathrm{gap}}$ and $D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] < -2(\mathrm{j}_1 - \mathrm{j}_3)$

$$D(\varrho)^2 = \min\Big\{\mathrm{j}_1 + \min\{0, -\frac{1}{2}D_{12}^{(+)} + x_3^2, -\frac{1}{2}D_{13}^{(+)} + x_2^2\}, \\ \mathrm{j}_2 + (|x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}})^2\Big\} \tag{51}$$

We would like to emphasize that the stratification of the states given by the Classes I–IV itemized above opens a new way to further detailed analysis that seems to be still feasible: the conditions appearing in (48–51) provide a natural classification for states of the bipartite system formed by qubits. Indeed, the suggested approach is to focus separately on each single fraction formed by any single Class taken out of all the Classes from I up to IV. The complementary classification appears when we analyze the right discord D_R and take into account the Bloch vector y and the operator R given by (3). The full classification coming from the analysis of D_L and D_R taken together distinguishes all the states having any kind of quantum correlations as being not classical-quantum and quantum-classical simultaneously. The detailed analysis of the Classes presented will be discussed in a separate paper as the subject needs an extra space to be discussed in full. However, in the next section below we give an exemplary analysis to illustrate the approach suggested above and an application of the Theorem 4.1.

5 Applications in the study of states space for the qubit bipartite system

In this section, we introduce another classification of states pointing out features that allow the simple expressions for $D(\varrho)$. We introduce the following class of states called the *regular states*. Let L be an operator which is assigned to the state ϱ by (3) and (1). We call a state ϱ *left regular* if at least one of the following conditions named below is satisfied:

(i) the operator L has got any degeneracy in its spectrum
(ii) $\mathsf{adj}I = 0$ or the commutativity condition is satisfied:

$$LP_{\mathsf{x}} - P_{\mathsf{x}}L = 0 \tag{52}$$

(iii) the function (4) assumes the value $D(\varrho)$ at the point

$$M_* = \mathbf{1}_3 - P_{\mathsf{x}_*}$$

where $\mathsf{x}_* = \mathsf{x}/\|\mathsf{x}\|$ with x being a left Bloch vector. A state ϱ is *right regular* if it satisfies at least one condition as written above except we now replace the operator L by the operator R and the left Bloch vector x by the right Bloch vector y. The regular states include the most popular in use X-states as they satisfy the condition (52). The states that do not satisfy both conditions in (ii) are, in principle, more difficult in use and we have not found in the literature examples of such states except an example given in [8]. The states satisfying (i) have not been discussed in the literature, either. Our attention will be focused on the states that satisfy the condition (iii). Among elements of this class one finds states that do not satisfy (ii). Any state ϱ characterized by (iii) has got its vector x 'coupled' or 'adhered' to the value of $D(\varrho)$ and therefore for the sake of convenience such states are called below *left self-adhered* (or *right self-adhered* in the case when R and y is considered). First of all, it arises a natural question: does exist any self-adhered state?

The existence of the self-adhered states

The existence of self-adhered states is not an obvious matter beyond the trivial case when $\sqrt{c} = 0$. The affirmative answer to this question is connected with the principle of the three large circles on S^2, and in particular the universal property of the function d described by Lemma 7. Hence, using (8) and (9), the example of a state ϱ that is left self-adhered can be constructed as follows: let L be chosen in an arbitrary way, except L has got a non-degenerate spectrum, then we select the Bloch vector in the form

$$\mathsf{x} = \|\mathsf{x}\| \left(\sqrt{t + (1-t)\frac{\tilde{\lambda}_1 - \tilde{\lambda}_2}{\tilde{\lambda}_1 - \tilde{\lambda}_3}},\ 0\ ,\ \sqrt{(1-t)\frac{\tilde{\lambda}_2 - \tilde{\lambda}_3}{\tilde{\lambda}_1 - \tilde{\lambda}_3}} \right) \tag{53}$$

where t is an auxiliary parameter chosen in the interval $[0, 1]$, arbitrarily. In the example under discussion we need to choose L and the value of $\|\mathsf{x}\|$ in a such a way that the positivity condition holds true for ϱ given by (1).

The analytical formula for the discord of the left self-adhered states[1]

Knowing that the state ϱ is left self-adhered the analytical formula for the discord $D(\varrho)$ can be easily obtained. In the equation (3.1) from [8], one can put $M_* = \mathbf{1} - \frac{1}{\|\mathsf{x}\|^2} P_{\mathsf{x}}$. Then $M_*\mathsf{x} = 0$, and introducing the normalized Bloch vector $\mathsf{x}_* \in \mathsf{S}^2$ by $\mathsf{x}_* = \frac{1}{\|\mathsf{x}\|}\mathsf{x}$ we obtain

$$\mathsf{Tr} M_* I I^T = \mathsf{Tr} I I^T - \|I^T \mathsf{x}_*\|^2 \quad \text{and} \quad \mathsf{Tr}(\mathbf{1} - M_*)\mathsf{adj}I^T \mathsf{adj}I = \|\mathsf{adj}I \mathsf{x}_*\|^2$$

Taking into account these expressions above, we get the following expression describing discord for the left self-adhered states

$$2D(\varrho)^2 = \mathsf{Tr} I I^T - \|I^T \mathsf{x}_*\|^2 + \sqrt{[\mathsf{Tr} I I^T - \|I^T \mathsf{x}_*\|^2]^2 - 4\|\mathsf{adj}I \mathsf{x}_*\|^2} \tag{54}$$

We notice that the norm of Bloch vector x does not play any role, and its direction given by x_* is significant only. The form of the admissible Bloch vectors x is described by the Propositions: 5.1, 5.2, 5.3 and 5.4, 5.5. We remark that the operators II^T and L do not commute in general, so in particular the coordinates of admissible vectors x_* in the formula (54) may have all their coordinates non-vanishing even when some of coordinates of x_* do vanish in the ordered basis formed from eigenvectors of L.

The classification of the left self-adhered states

As an example of possible applications of our analysis given in the Sect. 4, we give now some quite complete description of all left self-adhered states. To get the full classification of such states, one needs to discuss in details two cases

(i) the spectrum of L is non-degenerate: under what condition is it possible that the Bloch vector x, satisfying one of the equations: $x_1 = 0$ or $x_2 = 0$ or $x_3 = 0$ in the ordered basis of eigenvectors of L, may determine the minimum of the function (4)?
(ii) the spectrum of L has got a degeneracy: when the Bloch vector x points out the minimum?

[1] The whole discussion of this section can be carried out for the right self-adhered states.

As we have seen the case (i) above is non-empty as the state ϱ given by (53) (and comments around it) supplies us with a such example. The case (ii) is much simpler to analyze as we do not need to apply the result of the Sect. 4. We describe the second case at the end of this section.

The left self-adhered state for a non-degenerate spectrum of L
the case $x_3 = 0$.

We use formulae from (27) to (30), and we put there $x_3 = 0$. Next we consider $\min\{\mu_1, \mu_{**}\} = \min\{\mathrm{j}_1, \mathrm{j}_2\}$. We show that the following estimate holds true

$$\mu_* \geq \min\{\mathrm{j}_1, \mathrm{j}_2\}$$

To this end we note that $D_{13}^{(+)} \geq 0$. Let be $\mathrm{j}_1 \geq \mathrm{j}_3$, then never happens $\frac{1}{2}D_{13}^{(+)}[\tan^2\varphi_{gap} - 1] < -(\mathrm{j}_1 - \mathrm{j}_3)$ hence

$$\mu_* = \mathrm{j}_2 + x_1^2 \sin^2\varphi_{\mathrm{gap}} \geq \min\{\mathrm{j}_1, \mathrm{j}_2\}$$

If $\mathrm{j}_1 < \mathrm{j}_3$, then $D_{13}^{(+)} = 0$ and the condition $\frac{1}{2}D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] \geq -(\mathrm{j}_1 - \mathrm{j}_3)$ leads to $0 \geq -(\mathrm{j}_1 - \mathrm{j}_3)$ or equivalently to $\mathrm{j}_1 \geq \mathrm{j}_3$ so we get a contrdiction. Hence

$$\mu_* = \mathrm{j}_1 - \frac{1}{2}D_{13}^{(+)} + x_2^2 = \mathrm{j}_1 + x_2^2 \geq \min\{\mathrm{j}_1, \mathrm{j}_2\}$$

and the number μ_* can be excluded from further considerations. The number μ_2 has got the representation

$$\mu_2 = \frac{1}{2}\left\{\mathrm{j}_1 + \mathrm{j}_2 - \sqrt{(\mathrm{j}_1 - \mathrm{j}_2)^2 + 4x_1^2x_2^2}\right\}$$

If $\mathrm{j}_1 \geq \mathrm{j}_2$, then

$$\mu_2 = \mathrm{j}_2 + \frac{1}{2}\left\{\mathrm{j}_1 - \mathrm{j}_2 - \sqrt{(\mathrm{j}_1 - \mathrm{j}_2)^2 + 4x_1^2x_2^2}\right\} < \mathrm{j}_2 = \min\{\mathrm{j}_1, \mathrm{j}_2\}$$

since the expression in the bracket is negative. In a similar way, if $\mathrm{j}_1 < \mathrm{j}_2$, then

$$\mu_2 = \mathrm{j}_1 + \frac{1}{2}\left\{\mathrm{j}_2 - \mathrm{j}_1 - \sqrt{(\mathrm{j}_1 - \mathrm{j}_2)^2 + 4x_1^2x_2^2}\right\} < \mathrm{j}_1 = \min\{\mathrm{j}_1, \mathrm{j}_2\}$$

As a summary, one can write

$$\min\{\mu_1, \mu_2, \mu_*, \mu_{**}\} = \frac{1}{2}\left\{\mathrm{j}_1 + \mathrm{j}_2 - \sqrt{(\mathrm{j}_1 - \mathrm{j}_2)^2 + 4x_1^2x_2^2}\right\} \tag{55}$$

On the other hand, according to the properties of the function d the value of the function $M \to \mu(M)$ at the point $\mathsf{v}_* = \frac{1}{\|\mathsf{x}\|}(x_1, x_2, 0)$ is equal to

$$\mu = \tilde{\lambda}_2 + \sqrt{a}\frac{x_2^2}{\|\mathsf{x}\|^2} \tag{56}$$

At the end, we compare the number given by (55) to the one given by (56). We claim that

$$\min\{\mu_1, \mu_2, \mu_*, \mu_{**}\} < \mu \quad \text{only if} \quad x_1 \neq 0 \tag{57}$$

We multiply each side of the inequality above by 2 to get an equivalent inequality

$$\tilde{\lambda}_1 + \tilde{\lambda}_2 + \|\mathsf{x}\|^2 - \sqrt{(\sqrt{a} + \|\mathsf{x}\|^2)^2 - 4\sqrt{a}x_2^2} < 2\tilde{\lambda}_2 + 2\sqrt{a}\frac{x_2^2}{\|\mathsf{x}\|^2}$$

or

$$\sqrt{a} + \|\mathsf{x}\|^2 - \sqrt{(\sqrt{a} + \|\mathsf{x}\|^2)^2 - 4\sqrt{a}x_2^2} < 2\sqrt{a}\frac{x_2^2}{\|\mathsf{x}\|^2}$$

On left-hand side, we transform into

$$\frac{4\sqrt{a}x_2^2}{\sqrt{a} + \|\mathsf{x}\|^2 + \sqrt{(\sqrt{a} + \|\mathsf{x}\|^2)^2 - 4\sqrt{a}x_2^2}} < 2\sqrt{a}\frac{x_2^2}{\|\mathsf{x}\|^2}$$

After obvious simplifications, we arrive at

$$\|\mathsf{x}\|^2 - \sqrt{a} < \sqrt{(\sqrt{a} + \|\mathsf{x}\|^2)^2 - 4\sqrt{a}x_2^2}$$

If now $\|\mathsf{x}\|^2 - \sqrt{a} < 0$, then (57) holds true. Let be below $\|\mathsf{x}\|^2 - \sqrt{a} \geq 0$. We square both sides, and after some manipulations we get

$$-2\sqrt{a}\|\mathsf{x}\|^2 < 2\sqrt{a}\|\mathsf{x}\|^2 - 4\sqrt{a}x_2^2$$

or

$$0 < 4\sqrt{a}\|\mathsf{x}\|^2 - 4\sqrt{a}x_2^2 = 4\sqrt{a}x_1^2$$

which ends the proof of (57) only if $x_1 \neq 0$. The inequality (57) says that we have to do with self-adhered states only when $x_1 = 0$. We get the following

Proposition 5.1 *Let the state ϱ be such that the spectrum of L has got no degeneracy in its spectrum and the Bloch vector x has got a vanishing coordinate $x_3 = 0$ in the ordered basis of eigenvectors of L. Then the state ϱ is a self-adhered state if and only if the coordinate x_1 vanishes.*

the case $x_1 = 0$.

As in the previous case, we use expressions from (27) up to (30) and there we insert now $x_1 = 0$. We start with the remark that in this case we always have got $\mu_{**} = \mathsf{j}_2 + x_3^2\cos^2\varphi_{\text{gap}}$. We show that

$$\mu_2 \geq \min\{\mu_1, \mu_{**}\}$$

what means that in the discussion below one can omit μ_2. Indeed, we take $\mathsf{j}_1 \geq \mathsf{j}_2$ then $\mu_2 = \mathsf{j}_2 + x_3^2$ and hence $\mu_2 \geq \mu_{**}$. If now $\mathsf{j}_1 < \mathsf{j}_2$, then $\mu_2 = \mathsf{j}_1 + x_3^2$, and so $\mu_2 \geq \mu_1$.

Let be $\mathsf{j}_1 \geq \mathsf{j}_3$, then noting that $D_{13}^{(+)} \geq 0$ we obtain $\mu_* = \mathsf{j}_2 + x_3^2\cos^2\varphi_{\text{gap}} = \mu_{**}$. If we assume the converse $\mathsf{j}_1 < \mathsf{j}_3$, then $D_{13}^{(+)} = 0$ and $\mu_* = \mathsf{j}_1 + x_2^2 \geq \mathsf{j}_1 = \mu_1$. Summing up

$$\mu_* \geq \min\{\mu_1, \mu_{**}\}$$

and the number μ_* can be excluded from the further analysis. On the other hand, we calculate the value assumed by the function $M \to \mu(M)$ at the point $\mathsf{v}_* = \frac{1}{\|\mathsf{x}\|}(0, x_2, x_3)$. We get

$$\mu = \tilde{\lambda}_1 = \mu_1 \geq \min\{\mu_1, \mu_{**}\}$$

As a conclusion, we can say that one has to do with self-adhered states when the following condition is satisfied $\mu_1 = \mu_{**}$ in other word we arrive at $x_2^2 + x_3^2\cos^2\varphi_{\text{gap}} = \sqrt{a}$. The discussion can be summed up in the statement:

Proposition 5.2 *Let ϱ be a self-adhered state such that L has got a non-degenerate spectrum and for the Bloch vector x there is $x_1 = 0$ in the ordered basis formed by eigenvectors of L, then*

$$\frac{x_2^2}{\sqrt{a}} + \frac{x_3^2}{\sqrt{c}} = 1$$

Choosing parameters x_2^2, x_3^2 and $\sqrt{a}$, $\sqrt{b}$ that satisfy the equality above and moreover small enough to guarantee the positivity condition of ϱ given by (1) one sees that this class of states with $x_1 = 0$ is not empty and rather much richer than the class with $x_3 = 0$.

the case $x_2 = 0$.

This case is most difficult to analyze. We note that it is enough to consider a situation when the inequality holds true $|x_3| > |x_1|\tan\varphi_{\text{gap}}$. If the opposite inequality takes place, then we arrive at the class of states described by (53). The assumption taken above means in particular that $x_3 \neq 0$, always, and as a matter of fact it can be rewritten in the equivalent form

$$x_3^2\cos^2\varphi_{\text{gap}} > x_1^2\sin^2\varphi_{\text{gap}} \tag{58}$$

Let us begin with determination of μ for $\mathsf{v}_* = \frac{1}{\|\mathsf{x}\|}(x_1, 0, x_3)$

$$\mu = \tilde{\lambda}_1 - \sqrt{c}\frac{x_1^2}{\|\mathsf{x}\|^2} \tag{59}$$

Using (58), we can get the estimate of the parameter above, i.e. knowing that $\sqrt{c}\frac{x_1^2}{\|\mathsf{x}\|^2} < \sqrt{a}$ we obtain

$$\tilde{\lambda}_2 < \mu \leq \tilde{\lambda}_1 \tag{60}$$

The inequalities (60) derived above and (58) allow us to a more effective analysis of equations from (27) up to (30). Indeed, we want to find $\mu = \min\{\mu_1, \mu_2, \mu_*, \mu_{**}\}$ and the condition (60) means that we can exclude μ_1. The condition (58) leads to the conclusion that always

$$\mu_{**} = \mathrm{j}_2 + (|x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}})^2 \le \mathrm{j}_2 + x_3^2\cos^2\varphi_{\mathrm{gap}} < \mathrm{j}_2 + x_3^2 = \mu_2$$

and this means, in turn, that we can omit μ_2 either. On the other hand, the inequality (58), together with the expresion for μ_* given by (20), reduces the condition for the state to be a self-adhered state into the form

$$\mu = \mu_* \le \mu_{**} \tag{61}$$

At first we assume that for the matrix entries of II^T in the basis formed by ordered eigenvectors of L there is $D_{13}^{(+)}[\tan\varphi_{\mathrm{gap}} - 1] \ge -2(\mathrm{j}_1 - \mathrm{j}_3)$. In that case, we get the equality $\mu_* = \mu_{**}$. i.e. we get the equality in the condition (61) that leads to

$$\sqrt{a} - \sqrt{c}\frac{x_1^2}{\|\mathsf{x}\|^2} = (|x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}})^2 \tag{62}$$

We notice that one can rewrite the left-hand side of this equality in the form

$$\frac{\sqrt{a}x_1^2 + \sqrt{a}x_3^2 - \sqrt{c}x_1^2}{\|\mathsf{x}\|^2} = \frac{\sqrt{a}x_3^2 - \sqrt{b}x_1^2}{\|\mathsf{x}\|^2}$$

and so (62) leads to

$$\frac{\sqrt{c}}{\|\mathsf{x}\|^2}(x_3^2\cos^2\varphi_{\mathrm{gap}} - x_1^2\sin^2\varphi_{\mathrm{gap}}) = (|x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}})^2$$

Since the right-hand side of the last expression is positive according to (58), one can simplify this equality and obtain

$$\frac{\sqrt{c}}{\|\mathsf{x}\|^2}(|x_3|\cos\varphi_{\mathrm{gap}} + |x_1|\sin\varphi_{\mathrm{gap}}) = |x_3|\cos\varphi_{\mathrm{gap}} - |x_1|\sin\varphi_{\mathrm{gap}}$$

or equivalently, changing the sides, one can write

$$|x_3|\left(\|\mathsf{x}\|^2 - \sqrt{c}\right)\cos\varphi_{\mathrm{gap}} = |x_1|\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)\sin\varphi_{\mathrm{gap}} \tag{63}$$

Using the last equality, one gets in particular that

$$\sqrt{c} \le \|\mathsf{x}\|^2 \quad \Leftrightarrow \quad \mathrm{j}_1 \le \mathrm{j}_3 + 2x_1^2 \tag{64}$$

At the end of this part of the analysis, we transform (63) by making the substitution $x_1^2 = \|\mathsf{x}\|^2 - x_3^2$ into the expression

$$x_3^2\left(\|\mathsf{x}\|^2 - \sqrt{c}\right)^2\cos^2\varphi_{\mathrm{gap}} = (\|\mathsf{x}\|^2 - x_3^2)\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2\sin^2\varphi_{\mathrm{gap}}$$

or

$$\frac{x_3^2}{\|\mathsf{x}\|^2} = \frac{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2\sin^2\varphi_{\mathrm{gap}}}{\left(\|\mathsf{x}\|^2 - \sqrt{c}\right)^2\cos^2\varphi_{\mathrm{gap}} + \left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2\sin^2\varphi_{\mathrm{gap}}}$$

and finally if we simplify the denominator we arrive at

$$\frac{x_3^2}{\|\mathsf{x}\|^2} = \frac{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2\sin^2\varphi_{\mathrm{gap}}}{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2 - 4\sqrt{c}\|\mathsf{x}\|^2\cos^2\varphi_{\mathrm{gap}}} \tag{65}$$

If $x_1 = 0$, then from (64) we get $\mathrm{j}_1 \le \mathrm{j}_3$. On the other hand, according to the assumption made in this part, i.e. $\frac{1}{2}D_{13}^{(+)}[\tan\varphi_{\mathrm{gap}} - 1] \ge -(\mathrm{j}_1 - \mathrm{j}_3)$, we infer that $\mathrm{j}_1 \ge \mathrm{j}_3$. Hence $x_1 = 0$ implies $\mathrm{j}_1 = \mathrm{j}_3$.

Let now be $D_{13}^{(+)}[\tan^2\varphi_{\mathrm{gap}} - 1] < -2(\mathrm{j}_1 - \mathrm{j}_3)$. In this case there is more conditions to be taken into account: besides $\mu = \mu_*$ it must be satisfied $\mu_* \le \mu_{**}$, as well. The last inequality can be replaced by $\mu \le \mu_{**}$ with keeping the condition $\mu = \mu_*$. It is convenient as it allows us to use the results from the previous part; in particular, we can assume now additionally that (64) holds true. The condition $\mu_* \le \mu_{**}$ can be rewritten at once as

$$\frac{x_3^2}{\|\mathsf{x}\|^2} \ge \frac{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2\sin^2\varphi_{\mathrm{gap}}}{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2 - 4\sqrt{c}\|\mathsf{x}\|^2\cos^2\varphi_{\mathrm{gap}}} \tag{66}$$

We are left with the equality $\mu = \mu_*$ to analyze. Let us write

$$\tilde{\lambda}_1 - \sqrt{c}\frac{x_1^2}{\|\mathsf{x}\|^2} = \tilde{\lambda}_1 + x_1^2 - \frac{1}{2}\left\{\mathrm{j}_1 - \mathrm{j}_3 + \sqrt{(\mathrm{j}_1 - \mathrm{j}_3)^2 + 4x_1^3x_3^2}\right\}$$

and hence

$$\mathrm{j}_3 - \mathrm{j}_1 + 2\left(1 + \frac{\sqrt{c}}{\|\mathsf{x}\|^2}\right)x_1^2 = \sqrt{(\mathrm{j}_1 - \mathrm{j}_3)^2 + 4x_1^3 x_3^2}$$

The left-hand side of the inequality is negative; otherwise, the condition $\mu = \mu_*$ is not fulfilled. We use this observation later. We express now the matrix entries of II^T by parameters related to L and x

$$-\sqrt{c} + x_3^2 + x_1^2 + 2\frac{\sqrt{c}}{\|\mathsf{x}\|^2}x_1^2 = \sqrt{(\sqrt{c} + x_1^2 - x_3^2)^2 + 4x_1^2 x_3^2}$$

The first and forth terms on the left-hand side of this equality can be put together, but on the right-hand side we rearrange the expression under the square root

$$\|\mathsf{x}\|^2 + \sqrt{c}\left(\frac{-x_1^2 - x_3^2 + 2x_1^2}{\|\mathsf{x}\|^2}\right) = \sqrt{\sqrt{c}^2 + (x_1^2 + x_3^2)^2 + 2\sqrt{c}(x_1^2 - x_3^2)}$$

or

$$\|\mathsf{x}\|^2 + \frac{\sqrt{c}}{\|\mathsf{x}\|^2}\left(x_1^2 - x_3^2\right) = \sqrt{\sqrt{c}^2 + \|\mathsf{x}\|^4 + 2\sqrt{c}(x_1^2 - x_3^2)}$$

Since the left-hand side is non-negative, we can square both sides of the last equality

$$\|\mathsf{x}\|^4 + \frac{\sqrt{c}^2}{\|\mathsf{x}\|^4}\left(x_1^2 - x_3^2\right)^2 + 2\sqrt{c}(x_1^2 - x_3^2) = \sqrt{c}^2 + \|\mathsf{x}\|^4 + 2\sqrt{c}(x_1^2 - x_3^2)$$

After reductions of identical terms, we get $\|\mathsf{x}\|^4 = (x_1^2 - x_3^2)^2$. This equation gives $x_1 = 0$ as $x_3 \neq 0$. The condition (66) is fulfilled automatically; however, $D_{13}^{(+)}[\tan\varphi_{\text{gap}} - 1] < -2(\mathrm{j}_1 - \mathrm{j}_3)$ reduces to the inequality $\mathrm{j}_3 > \mathrm{j}_1$ with the assumption $x_1 = 0$ kept. One can directly verify that in the case when $x_1 = 0$ one gets $\mu = \mu^* = \tilde{\lambda}_1 < \tilde{\lambda}_2 + x_3^2\cos^2\varphi_{\text{gap}} = \mu_{**}$ as it should be since keeping $x_1 = 0$ with the present regime, the condition $D_{13}^{(+)}[\tan\varphi_{\text{gap}} - 1] \geq -2(\mathrm{j}_1 - \mathrm{j}_3)$, that guarantees the equality $\mu_* = \mu_{**}$, reduces to $\mathrm{j}_1 - \mathrm{j}_3 \geq 0$, i.e. to the opposite condition to the one desired presently. In summary of this part of discussion, the case $x_1 = 0$ with $\mathrm{j}_3 > \mathrm{j}_1$ kept is admissible since (64) should be satisfied as it takes place exactly. As a result of this, reasoning presented above we can formulate the following:

Proposition 5.3 *Let ϱ be a self-adhered state such that the corresponding L has got a non-degenerate spectrum and $x_2 = 0$ vanishes in the ordered basis formed by eigenvectors of L, then the Bloch vector x is given by (53) or satisfies $j_1 \leq j_3 + 2x_1^2$ and additionally*

$$\frac{x_3^2}{\|\mathsf{x}\|^2} = \frac{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2 \sin^2\varphi_{\text{gap}}}{\left(\|\mathsf{x}\|^2 + \sqrt{c}\right)^2 - 4\sqrt{c}\|\mathsf{x}\|^2\cos^2\varphi_{\text{gap}}} \quad \textit{if} \quad D_{13}^{(+)}\tan^2\varphi_{\text{gap}} \geq D_{13}^{(-)}$$

$$x_1 = 0 \quad \textit{if} \quad j_1 < j_3$$

This class of states described above is non-empty as one can consider small enough parameters of L and x to secure the positivity condition of ϱ described by (1).

The left self-adhered state for a degenerate spectrum of L

If L has got degeneracy described by the condition $\sqrt{a} = 0$ and $\sqrt{b} \neq 0$. Then

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

and the minimu is assumed if and only if v is parallel to x. In the case of the full degeneracy of the spectrum of L, i.e. when $\sqrt{c} = 0$, we have to do with self-adhered states in an obvious way. We get:

Proposition 5.4 *If for the state ϱ the operator L has got a degeneracy of spectrum described by the condition $\sqrt{a} = 0$, then ϱ is left self-adhered.*

If the Bloch vector x is a eigenvector of the operator $\sqrt{a}P_{(1,0,0)} + P_{\mathsf{x}}$, then it determines the direction at which the function (4) assumes its minimum value. It means that the vector x satisfies one of the following conditions: $\mathsf{x} = (x_1, 0, 0)$ or $\mathsf{x} = (0, x_2, x_3)$. Let us consider the first case then v_* at which the function (4) assumes its minimum needs to have the form $\mathsf{v}_* = (1, 0, 0)$ and then one gets

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

On the other hand, $D(\varrho)^2 = \tilde{\lambda}_2$ from Theorem 3.2 and so the state ϱ is left self-adhered. Next we consider the second possibility and put $\mathsf{v}_* = \frac{1}{\|\mathsf{x}\|}(0, x_2, x_3)$ where $\|\mathsf{x}\| = \sqrt{x_2^2 + x_3^2}$. Then as previously

$$\mu = \tilde{\lambda}_1 + \|\mathsf{x}\|^2 - \|\mathsf{x}\|^2 = \tilde{\lambda}_1$$

This value we compare to $D(\varrho)^2$ given by Theorem 3.2. We notice that $\mu > D(\varrho)^2$ only if

$$\sqrt{a} > \|\mathsf{x}\|^2 - \sqrt{(\sqrt{a} + \|\mathsf{x}\|^2)^2 + 4\sqrt{a}\|\mathsf{x}\|^2}$$

But the last inequality holds true as the following one

$$\sqrt{a} > \|\mathsf{x}\|^2 - \sqrt{(\sqrt{a} + \|\mathsf{x}\|^2)^2}$$

holds true in an obvious way. Summing up, v_* is not the point at which the function (4) assumes its minimum and consequently, the state ϱ is not a left self-adhered. We have proven:

Proposition 5.5 *If the operator L related to the state ϱ possesses a degeneracy given by $\sqrt{a} \neq 0$ and $\sqrt{b} = 0$, then the state ϱ is left self-adhered if and only if $x_2 = x_3 = 0$ for the Bloch vector x given in the ordered basis of eigenvectors of L.*

These states belong to the class (ii) of the definition of the regular states. We end the discussion with the following remark:

Remark 5.1 One can repeat the analysis above to get the characterisation for the class of right self-adhered states.

6 Summary

One of the main goals set in the present article is to clarify the results published in [8] and make them more manageable in further potential applications. This aim has been achieved in a twofold way. First of all, we would like to emphasize that one of the most difficult issues of the whole analysis is concentrated around the principle of the three large circles proposed in [8] and its justification. The rigorous proof of this principle provided here by us is a non-trivial step to achieve a better insight into the problem how to compute the discord $D(\varrho)$. Our novel approach to treat the three large circles principle is based on a geometrical argument with the use of two horizontal fields: one for the base function d and one for its perturbation $-\langle \mathsf{x}, \mathsf{v}\rangle^2$. Consequently, the exceedingly complex algebraic reasoning sketched in [8] with many tricky formulae involved is no longer needed and can be abandoned entirely. On the other hand, the expressions for the discord $D(\varrho)$ given in the previous paper can be seen just as a kind of knowledge which tells what can be done in principle, but the suggested practical way to realize is rather ineffective mainly due to the unintuitive and unhandy special functions used, p_L and r_L, that appear in various auxiliary formulae. In this regard, the main result of our paper, i.e., Theorem 4.1, brings a progress despite all the final complexity it bears: the new formula obtained for the discord $D(\varrho)$ is more concise having no reference to the special functions mentioned and hence it became far more tractable as given previously. There is a little hope to make it better as the matter of analysis reveals its sophistication. However, we point out that this theorem opens some new possibilities in study of the space of all states for two qubits which, in turn, is still not recognized in full. Indeed, as we have demonstrated above, the main result of the present paper can be helpful to classify all states where one can focus at the distinguished subgroups subjected to a special conditions that can be separately investigated in details. In particular, we have established the existence and gave a full mathematical classification of the self-adhered states ϱ for which the value of $D(\varrho)$ is straightforwardly connected with the direction of its Bloch vector. This led us to a recognition of new classes of states accordingly giving a contribution to the description of the space of all states for two qubits. More generally, we have highlighted the regular states as these for which the formula giving $D(\varrho)$ is relatively simple. In this class, among the X-states extensively used in the main course of research, one finds the self-adhered states considered for the first time.

The discussion carried out in our article shows clearly that there exists a wide class of states being not recognized until now and exhibiting interesting features that need to be examine. The presented analysis and the novel perspective proposed here provide a step to obtain new tools for deepening a mathematical research on the space of states for the system of two qubits.

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