Generalized Bloch Vector and the Eigenvalues of a Density Matrix

Māris Ozols Laura Mančinska

Institute of Mathematics and Computer Science,
University of Latvia, Raiņa bulv. 29, Rīga, LV-1459, Latvia.

Abstract

We consider n-level quantum systems and show how the length of the generalized Bloch vector is related to the eigenvalues of the density matrix. We interpret the length of the generalized Bloch vector as a measure of how pure the quantum state is.

1 Introduction

There is a one-to-one correspondence between the states of a 2-level quantum system (*qubit*) and the points of a unit ball in $\mathbb{R}^3$ – the *Bloch ball* (we will discuss this correspondence in Section 2.1). It has been generalized to systems with arbitrary number of levels (see Section 2.2 for 3-level system (*qutrit*) and Section 2.3 for general case). Unfortunately for quantum systems with more than 2 levels (qutrit, for example) the correspondence is not so clear anymore as in the qubit case, because the subset of points of the Bloch ball that correspond to valid quantum states has a nontrivial shape [6]. But still the Bloch vectors provide a visual insight into the world of quantum states.

We study the length of the generalized Bolch vector as a function of the eigenvalues of the density matrix in the qubit (Section 3.1), qutrit (Section 3.2) and the case of n-level quantum system for arbitrary n (Section 3.3). We demonstrate the spherical symmetry and linearity of this function (Section 4) and interpret it as a measure of how pure a quantum state is (Section 5).

2 The Bloch Vector

2.1 Qubit Case

In the qubit case the Bloch vectors span the entire unit ball in $\mathbb{R}^3$. Thus any point $\mathbf{r} = (x, y, z)$ with $|\mathbf{r}| \leq 1$ corresponds to a valid qubit state (this is not true for qutrits, see Section 2.2). Such points are given by

$$\begin{cases} x = r \sin\theta \cos\varphi \\ y = r \sin\theta \sin\varphi \\ z = r \cos\theta, \end{cases} \tag{1}$$

where $0 \leq \theta \leq \pi$, $0 \leq \varphi < 2\pi$ and $0 \leq r \leq 1$. Points on the surface ($|\mathbf{r}| = 1$) correspond to *pure qubit states*. Points with $|\mathbf{r}| < 1$ correspond to *mixed states* (the origin $\mathbf{r} = 0$ corresponds to *completely mixed state*).

If $|\mathbf{r}| = 1$, the pure state $|\psi\rangle$ that corresponds to $\mathbf{r}$ is given by

$$|\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix}. \tag{2}$$

The *density matrix* ρ of a pure state $|\psi\rangle$ is given by $\rho = |\psi\rangle\langle\psi|$. According to (1) and (2) we have:

$$\rho = \frac{1}{2}\begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix} = \frac{1}{2}(I + x\sigma_x + y\sigma_y + z\sigma_z), \tag{3}$$

where I is the identity matrix, but

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4}$$

are the *Pauli matrices*. Introducing a formal vector $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, equation (3) can be written as

$$\rho = \frac{1}{2}(I + \mathbf{r}\cdot\sigma). \tag{5}$$

The density matrix ρ of a mixed state is a probabilistic mixture of matrices ρ_i of pure states: $\rho = \sum_{i=1}^{k} c_i\rho_i$, where $0 \leq c_i \leq 1$ and $\sum_{i=1}^{k} c_i = 1$. Observe that according to (5) the Bloch vector $\mathbf{r}$ that corresponds to ρ is a linear combination of vectors $\mathbf{r}_i$ that correspond to matrices ρ_i: $\mathbf{r} = \sum_{i=1}^{k} c_i\mathbf{r}_i$. It means, (5) holds for mixed states as well. It provides a one-to-one correspondence between qubit states and points of unit ball in $\mathbb{R}^3$.

2.2 Qutrit Case

In the qutrit case one has to use the *Gell-Mann matrices* λ_i instead of the Pauli matrices σ_i (4) to specify a general qutrit density matrix [1, 2]:

$$\rho = \frac{1}{3}(I + \sqrt{3}\,\mathbf{r}\cdot\lambda), \tag{6}$$

where $\mathbf{r} \in \mathbb{R}^8$ is the Bloch vector of qutrit state ρ and λ is a formal vector that consists of the Gell-Mann matrices:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{7}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{8}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

For pure qutrit states Bloch vectors satisfy $|\mathbf{r}| = 1$, but for mixed states: $|\mathbf{r}| < 1$. However not all Bloch vectors with $|\mathbf{r}| \leq 1$ correspond to valid qutrit states (a valid state has density matrix with non-negative eigenvalues). For example, the Bloch vector $\mathbf{r} = (0, 0, 0, 0, 0, 0, 0, 1)$ is not associated with a valid qutrit state, because the density matrix (6) has eigenvalues $2/3$, $2/3$ and $-1/3$.

2.3 General Case

In a way similar to qubit and qutrit cases one can define the Bloch vector for n-level systems where $n \geq 3$. For example, the 4-level system (two qubits) has been studied in [3]. To define a generalized Bloch vector we will follow [4] with a different sign convention (as in [5]) to precisely obtain the Pauli and Gell-Mann matrices for cases $n = 2$ and $n = 3$ respectively.

Let $\{|1\rangle, |2\rangle, \ldots, |n\rangle\}$ be an orthonormal base of n-level system. Let us define a set of n^2 projection operators

$$P_{jk} = |j\rangle \langle k|, \tag{9}$$

where $j, k \in \{1, 2, \ldots, n\}$. Each operator P_{jk} has only one non-zero matrix element $(P_{jk})_{jk} = 1$. Let us construct a set of $n - 1$ diagonal operators

$$w_j = \sqrt{\frac{2}{j(j+1)}} \left(P_{11} + P_{22} + \cdots + P_{jj} - j \cdot P_{j+1,j+1}\right), \tag{10}$$

where $1 \leq j \leq n - 1$ and two sets of $n(n-1)/2$ operators in each

$$u_{jk} = P_{kj} + P_{jk}, \tag{11}$$

$$v_{jk} = i(P_{kj} - P_{jk}), \tag{12}$$

where $1 \leq j < k \leq n$. The set $\{\lambda_i\} = \{w_j\} \cup \{u_{jk}\} \cup \{v_{jk}\}$ consists of $n^2 - 1$ operators and matrices λ_i are called *generalized Pauli matrices* or SU(n) *generators* [4, 5, 6, 7, 8]. They satisfy the following relations:

$$\mathrm{Tr}(\lambda_i) = 0, \tag{13}$$

$$\mathrm{Tr}(\lambda_i \lambda_j) = 2\delta_{ij}. \tag{14}$$

Any density matrix ρ can be expressed as a linear combination of matrices λ_i:

$$\rho = \frac{1}{n} \left(I + \sqrt{\frac{n(n-1)}{2}}\, \mathbf{r} \cdot \lambda \right), \tag{15}$$

where $\mathbf{r} = (x_1, x_2, \ldots, x_{n^2-1}) \in \mathbb{R}^{n^2-1}$ is the *generalized Bloch vector* or *coherence vector* [4, 6, 7, 8]. Some authors [4, 6, 7] do not normalize the coefficients x_i in (15), thus the radius of the Bloch ball depends on dimension n. We follow [8] and normalize them, therefore the Bloch ball is a unit ball in all dimensions n. An additional benefit of normalization is that (15) matches (6) for $n = 3$.

It is known that there are no valid states such that $|\mathbf{r}| > 1$. Pure states have $|\mathbf{r}| = 1$, but mixed states have $|\mathbf{r}| < 1$. However not all Bloch vectors with $|\mathbf{r}| \leq 1$ correspond to valid states. It is known [7] that the largest ball, that contains only valid states, has radius $|\mathbf{r}| = 2/n$.

3 The Length of the Bloch Vector

In this section we will express the length of the Bloch vector $\mathbf{r}$ in terms of the eigenvalues of density matrix (15). First we will consider the qubit and qutrit cases and then proceed to the general case.

3.1 Qubit Case

To find the eigenvalues τ of the density matrix ρ given by (3), we must solve $\det(\tau I - \rho) = 0$, where $\det(\tau I - \rho)$ is the *characteristic polynomial*[1] of ρ:

$$\tau^2 - \tau + \frac{1}{4}(1 - |\mathbf{r}|^2) = 0. \tag{16}$$

Observe that (16) can be written as

$$(\tau - \tau_1)(\tau - \tau_2) = \tau^2 - (\tau_1 + \tau_2)\tau + \tau_1\tau_2, \tag{17}$$

where τ_1 and τ_2 are the roots of (16) or the eigenvalues of ρ. From (16) and (17) we get $\tau_1\tau_2 = (1 - |\mathbf{r}|^2)/4$ or

$$|\mathbf{r}|^2 = 1 - 4\tau_1\tau_2. \tag{18}$$

For pure states we have $\tau_1 = 1$, $\tau_2 = 0$ and $|\mathbf{r}| = 1$, but for completely mixed state we have $\tau_1 = \tau_2 = 1/2$ and $\mathbf{r} = 0$. In both cases our result agrees with definitions in Section 2.1.

3.2 Qutrit Case

The characteristic polynomial of (6) is (see also [6])

$$\begin{aligned}\tau^3 - \tau^2 + \frac{1}{3}(1 - |\mathbf{r}|^2)\tau + \frac{1}{9}(1 + x_8)\,|\mathbf{r}|^2 + \frac{2}{3\sqrt{3}}(x_2x_4x_6 - x_1x_2x_3 - x_3x_4x_5 - x_1x_5x_6) \\ + \frac{1}{3\sqrt{3}}(x_3^2 - x_2^2 + x_6^2 - x_5^2)x_7 - \frac{1}{3}(x_1^2 + x_4^2 + x_7^2)x_8 - \frac{1}{27}(1 + x_8^3) = 0.\end{aligned} \tag{19}$$

If τ_1, τ_2, τ_3 are the roots of (19), we can write it as

$$(\tau - \tau_1)(\tau - \tau_2)(\tau - \tau_3) = \tau^3 - (\tau_1 + \tau_2 + \tau_3)\tau^2 + (\tau_1\tau_2 + \tau_2\tau_3 + \tau_3\tau_1)\tau - \tau_1\tau_2\tau_3. \tag{20}$$

Coefficients for τ must be the same in (19) and (20), therefore

$$|\mathbf{r}|^2 = 1 - 3(\tau_1\tau_2 + \tau_2\tau_3 + \tau_3\tau_1). \tag{21}$$

3.3 General Case

In the qubit case the equation (18) for $|\mathbf{r}|^2$ was obtained by considering the coefficient at τ^0 in (16). In qutrit case equation (21) was obtained by considering the coefficient at τ^1 in (19). In the general case the characteristic polynomial is

$$\det(\tau I - \rho) = \tau^n + c_1\tau^{n-1} + c_2\tau^{n-2} + \cdots + c_{n-1}\tau + c_0 \tag{22}$$

[1] Some authors use $\det(\rho - \tau I)$ instead [8, 9].

and we will consider the coefficient c_2 at τ^{n-2}. It is given by [9], see also [8]:

$$c_2 = \frac{1}{2}\left((\operatorname{Tr}\rho)^2 - \operatorname{Tr}(\rho^2)\right) = \frac{1}{2}\left(1 - \operatorname{Tr}(\rho^2)\right), \tag{23}$$

because for density matrices $\operatorname{Tr}\rho = 1$. According to [8] we have:

$$\operatorname{Tr}(\rho^2) = \frac{1}{n}\left(1 + (n-1)\,|\mathbf{r}|^2\right) \tag{24}$$

and

$$c_2 = \frac{n-1}{2n}(1 - |\mathbf{r}|^2). \tag{25}$$

Let $\{\tau_1, \tau_2, \ldots, \tau_n\}$ be the roots of (22) and thus the eigenvalues of ρ. We can express c_2 also as

$$c_2 = \sum_{1\le i<j\le n} \tau_i \tau_j = P_2(\tau_1, \tau_2, \ldots, \tau_n), \tag{26}$$

where P_2 is the second order symmetric polynomial of n variables. From equations (25) and (26) we obtain the following result:

Theorem 1. *The Bloch vector* $\mathbf{r}$ *of n-level system satisfies*

$$|\mathbf{r}|^2 = 1 - \frac{2n}{n-1} P_2(\tau_1, \tau_2, \ldots, \tau_n), \tag{27}$$

where τ_i are the eigenvalues of the density matrix ρ that corresponds to $\mathbf{r}$.

For $n = 2$ and $n = 3$ the equation (27) matches (18) and (21) respectively. One can deduce from the Lemma proved in Appendix A that $0 \le |\mathbf{r}| \le 1$ and $|\mathbf{r}| = 0$ only if $\forall i : \tau_i = 1/n$ that corresponds to completely mixed state. It is not hard to verify that $|\mathbf{r}| = 1$ only if $\exists i : \tau_i = 1$ that corresponds to pure state.

However we can significantly simplify (27) using the following relation:

$$1^2 = (\tau_1 + \tau_2 + \cdots + \tau_n)^2 = \tau_1^2 + \tau_2^2 + \cdots + \tau_n^2 + 2P_2(\tau_1, \tau_2, \ldots, \tau_n). \tag{28}$$

Let $\tau = (\tau_1, \tau_2, \ldots, \tau_n)$. We can express the symmetric polynomial as

$$P_2(\tau_1, \tau_2, \ldots, \tau_n) = \frac{1}{2}(1 - |\tau|^2), \tag{29}$$

thus (27) is the same as

$$|\mathbf{r}|^2 = \frac{n}{n-1}\left(|\tau|^2 - \frac{1}{n}\right). \tag{30}$$

One can find $|\mathbf{r}|^2$ also without knowing the eigenvalues τ_i, but using only the density matrix ρ. From (23), (25) and (30) we find that $|\tau|^2 = \operatorname{Tr}(\rho^2)$.

If the Bloch vector is not normalized to fit inside the unit ball as in [4, 6, 7], the expressions (27) and (30) are given by:

$$|\mathbf{r}|^2 = \frac{2(n-1)}{n} - 4P_2(\tau_1, \tau_2, \ldots, \tau_n) = 2\left(|\tau|^2 - \frac{1}{n}\right). \tag{31}$$

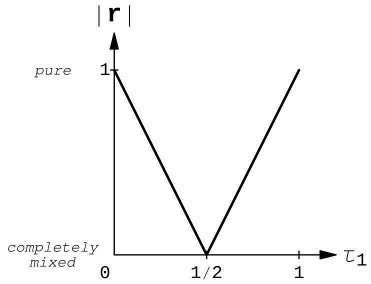

Figure 1: The length of the Bloch vector $|\mathbf{r}|$ for qubit as a function of the eigenvalue τ_1.

4 Linearity and Spherical Symmetry

It is obvious that $|\mathbf{r}|$ is spherically symmetric and linear in the space of Bloch vectors $\mathbf{r} = (x_1, x_2, \ldots, x_{n^2-1}) \in \mathbb{R}^{n^2-1}$. In this section we will show that the same holds in the space of eigenvalues $\tau = (\tau_1, \tau_2, \ldots, \tau_n) \in \mathbb{R}^n$, i.e. $|\mathbf{r}|$ is proportional to the distance between points τ and $\nu = (1/n, 1/n, \ldots, 1/n)$.

Let us consider the qubit case as an example. In the qubit case we have $\tau_1 + \tau_2 = 1$. If we put $\tau_2 = 1 - \tau_1$ into (18), we obtain $|\mathbf{r}| = |2\tau_1 - 1|$. It means, $|\mathbf{r}|$ changes linearly from 0 to 1 as τ_1 goes from 1/2 to 1 (see Fig. 1).

A similar linearity can be observed in the qutrit case as well. In order to visualize it, we will assign a point $\tau = (\tau_1, \tau_2, \tau_3) \in \mathbb{R}^3$ to each set of eigenvalues. The obtained region is a regular triangle shown in Fig. 2. We will call it the *eigenvalue simplex*. Despite the fact that in the qutrit case it is two-dimensional, at each point the three-element set (τ_1, τ_2, τ_3) is uniquely determined (because $\tau_1 + \tau_2 + \tau_3 = 1$). Therefore to each point a unique length of the generalized Bloch vector given by (21) can be assigned. The surface obtained in this way is shown in Fig. 3. It clearly exhibits the linear dependence of $|\mathbf{r}|$ on τ_i, i.e. no matter in which direction in the eigenvalue simplex one walks away form the midpoint $(1/3, 1/3, 1/3)$ of the triangle (shown in Fig. 2 and Fig. 3), the length of the Bloch vector $|\mathbf{r}|$ changes linearly and with the same ratio. We will prove that this property holds for any n, i.e.

Theorem 2. *The length of the Bloch vector $|\mathbf{r}|$ for state ρ is proportional to the distance between $\tau = (\tau_1, \tau_2, \ldots, \tau_n)$ and $\nu = (1/n, 1/n, \ldots, 1/n)$ in the eigenvalue simplex, where τ_i are the eigenvalues of ρ.*

Proof. Let $\delta = \tau - \nu$, where $\nu = (1/n, 1/n, \ldots, 1/n)$ corresponds to completely mixed state. Observe that $\tau_1 + \tau_2 + \cdots + \tau_n = 1$ implies

$$\delta_1 + \delta_2 + \cdots + \delta_n = 0. \tag{32}$$

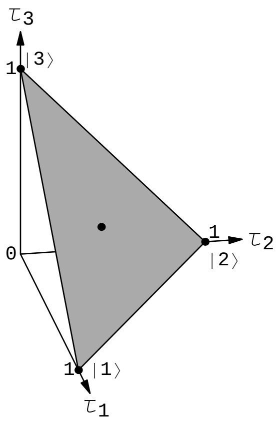

Figure 2: The eigenvalue simplex of the qutrit – all points (τ_1, τ_2, τ_3), such that $0 \leq \tau_i \leq 1$ and $\tau_1 + \tau_2 + \tau_3 = 1$. The corners of the triangle correspond to pure states $|1\rangle$, $|2\rangle$, $|3\rangle$, but the midpoint - to completely mixed state.

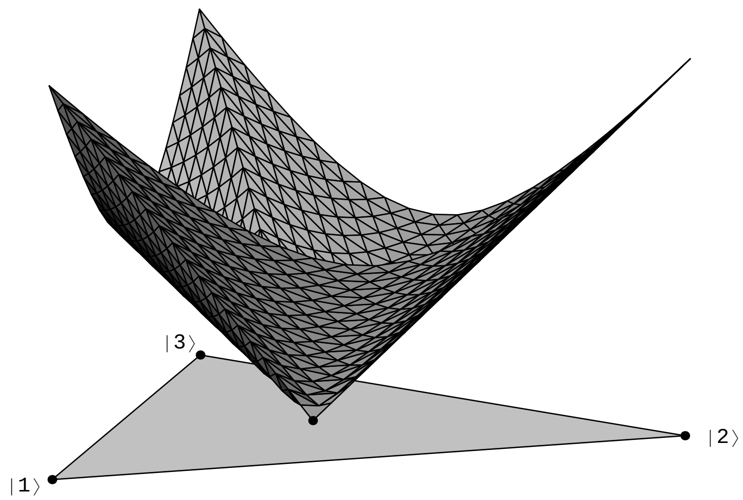

Figure 3: The length of the Bloch vector $|\mathbf{r}|$ (on z-axis) as a function of the eigenvalues τ_1, τ_2, τ_3 according to (21). The graph is plotted on the triangle shown in Fig. 2. It is a section of a cone and a triangular cylinder.

According to (30) we have

$$|\mathbf{r}|^2 = \frac{n}{n-1}\left(|\delta+\nu|^2 - \frac{1}{n}\right) = \frac{n}{n-1}\left(\sum_{i=1}^{n}\left(\delta_i + \frac{1}{n}\right)^2 - \frac{1}{n}\right) =$$

$$= \frac{n}{n-1}\left(\sum_{i=1}^{n}\delta_i^2 + 2\frac{1}{n}\sum_{i=1}^{n}\delta_i + n\frac{1}{n^2} - \frac{1}{n}\right) = \frac{n}{n-1}|\delta|^2, \quad (33)$$

where (32) was used to obtain the last equality. Finally we obtain

$$|\mathbf{r}| = \sqrt{\frac{n}{n-1}}\,|\tau-\nu|\,. \quad (34)$$

It means $|\mathbf{r}|$ is spherically symmetric in the eigenvalue simplex with the center of symmetry being the point ν and it changes linearly in any direction. □

5 Conclusion

We obtained an expression for the length of the generalized Bloch vector $\mathbf{r}$ of the n-level quantum system as a function of the eigenvalues of the density matrix ρ. In the qubit and qutrit cases it is given by (18) and (21) respectively, but in general case – by (30).

In Section 3.3 we concluded that $0 \le |\mathbf{r}| \le 1$ and for completely mixed state we have $|\mathbf{r}| = 0$, but for pure states we have $|\mathbf{r}| = 1$. This suggests that the length of the generalized Bloch vector $\mathbf{r}$ can be used to measure the *purity* of the corresponding quantum state ρ, i.e. how pure the state ρ is.

In Section 4 we showed that $|\mathbf{r}|$ is spherically symmetric in the eigenvalue simplex around the point ν that corresponds to the completely mixed state and changes linearly in any direction. Equation (34) provides a natural interpretation of the purity – it is the distance in the eigenvalue simplex between τ and the point ν that corresponds to the completely mixed state, where $\tau = (\tau_1, \tau_2, \ldots, \tau_n)$ are the eigenvalues of the density matrix ρ.

A Appendix: Inequality

To see, how large and how small $|\mathbf{r}|$ can be in equation (27) and for what values of τ_i these extremes are obtained, we will prove the following lemma:

Lemma 1. *For all $\tau_1, \tau_2, \ldots, \tau_n$, $n \ge 2$ such that $0 \le \tau_i \le 1$ and $\sum_{i=1}^{n}\tau_i = 1$*

$$0 \le P_2(\tau_1, \tau_2, \ldots, \tau_n) \le \frac{n-1}{2n}. \quad (35)$$

Proof. The first inequality is obvious – we will prove only the second. For $n = 2$ we have $0 \le (\tau_1-\tau_2)^2 = (\tau_1+\tau_2)^2 - 4\tau_1\tau_2 = 1 - 4\tau_1\tau_2$. Therefore $\tau_1\tau_2 \le 1/4$ and equality is reached only when $\tau_1 = \tau_2 = 1/2$. We will assume that (35) holds for $n = k-1$ and prove that it holds for $n = k$ as well. Let us fix $s = \tau_1 + \tau_2 + \cdots + \tau_{k-1}$. Then $\tau_k = 1 - s$ and

$$P_2(\tau_1, \tau_2, \ldots, \tau_k) = \sum_{1\le i<j\le n}^{k-1}\tau_i\tau_j + \tau_k\sum_{i=1}^{k-1}\tau_i = s^2 P_2\left(\frac{\tau_1}{s}, \frac{\tau_2}{s}, \ldots, \frac{\tau_{k-1}}{s}\right) + (1-s)s.$$

According to our assumption we obtain

$$P_2(\tau_1, \tau_2, \ldots, \tau_k) \leq s^2 \frac{k-2}{2(k-1)} + (1-s)s = -s^2 \frac{k}{2(k-1)} + s. \qquad (36)$$

The maximum of (36) is reached at $s = (k-1)/k$ and equals to $(k-1)/2k$. $\square$

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