

How many orthonormal bases are needed to distinguish all pure quantum states?

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Received 13 April 2015 / Received in final form 27 May 2015

1 Introduction

How many different measurement settings are needed in order to uniquely determine a pure quantum state, and how should such measurements be chosen? This problem goes back to a famous remark by Pauli [1], in which he raised the question whether or not the position and the momentum distributions are enough to define the wave function uniquely modulo a global phase. The original *Pauli problem* has a negative answer [2], but it has evolved into many interesting variants and has been studied from several fruitful perspectives. Discussion of the vast literature lies outside the scope of this work. Instead, we will concentrate only on a specific form of the Pauli problem, which is concerned with the minimal number of orthonormal bases, or projective measurements, in a finite dimensional Hilbert space that is needed in order to distinguish all pure quantum states. The purpose of this paper is to present the essential results related to our question in a comprehensible way.

It should be emphasized that in our treatment we require that *all* pure states are determined, so schemes that allow the determination of merely almost all pure states are outside of the scope of this work. Similarly, we are interested only in the case where the measurement settings are fixed, and therefore we do not consider adaptive schemes where the statistics of a given measurement may affect the choice of the subsequent measurement settings. Such schemes are interesting in their own right, as well as important from the practical point of view. Results in this direction, including an experimental demonstration, are presented e.g. in reference [3].

It is quite obvious that a single orthonormal basis cannot distinguish all pure states in a d -dimensional Hilbert space, while it is known that with $d + 1$ bases it is possible to distinguish all states, pure or mixed. The problem of finding the minimal number of orthonormal bases determining an unknown pure state has been raised several times in the past. It is easy to verify that the minimal number is three in dimension 2, but in higher dimensions the problem becomes more difficult. In 1978 Vogt reported on Wright's conjecture that three orthonormal bases are sufficient to identify an unknown pure state in any finite dimension [4]. In 1983 Moroz made the same claim and presented a proof for it [5], but in the erratum he explains that his proof does not work for all pure states and credits Gromov for pointing out an argument that shows that at least four bases are needed in large dimensions [6,7]. In 1994 this argument was spelled out in greater detail by Moroz and Perelomov [8], and they concluded that at least four bases are needed for any dimension $d \geq 9$. We will see that this conclusion can be extended to all dimensions $d \geq 5$ as a direct implication of the result of [9]. The sufficiency of four generic orthonormal bases for unique pure state determination was found by Mondragon and Voroninski [10], and a concrete method for constructing four bases with the desired property was recently introduced by Jaming [11].

This paper is organized as follows. We start by giving a precise mathematical formulation of the question in Section 2. In Section 3 we give an elementary argument for the fact that two orthonormal bases cannot distinguish all pure states in any dimension d . Then in Section 4 we review the rank criterion first found in reference [9] and explain how this implies that three bases are not enough in dimension 3. In Section 5 we give a thorough presentation

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of Jaming's construction of four bases. We continue in Section 6 with the most technical part of this paper, which reviews the argument presented in reference [9] that implies the impossibility of three bases in dimensions $d \geq 5$.

All these results together mean that the minimal number of orthonormal bases that are able to distinguish all pure quantum states is:

- three for $d = 2$;
- four for $d = 3$ and all dimensions $d \geq 5$;
- either three or four in $d = 4$.

Curiously, the final answer in $d = 4$ still remains open. In Section 7 we rule out specific types of triples of bases, namely, those consisting solely of product vectors with respect to a splitting of the Hilbert space into a tensor product of 2-dimensional spaces. Finally, in Section 8 we treat spin-1 measurements to highlight the fact that even if four bases can distinguish all pure quantum states, these bases must be chosen appropriately and it may happen that some natural choices are not the best ones. We end this paper with a brief discussion of the problem in an infinite dimensional Hilbert space in Section 9.

2 Formulation of the question

Let \mathcal{H} be a finite d -dimensional Hilbert space. The quantum states are described by density matrices, i.e., positive operators ρ on \mathcal{H} that satisfy $\text{tr}[\rho] = 1$. A quantum state ρ is *pure* if it cannot be written as a mixture $\rho = \frac{1}{2}\rho_1 + \frac{1}{2}\rho_2$ of two different states ρ_1 and ρ_2 . Pure quantum states correspond to 1-dimensional projections. They can be alternatively described as rays of vectors in \mathcal{H} , meaning that two vectors ψ_1 and ψ_2 correspond to the same pure state if there is a nonzero complex number c such that $\psi_1 = c\psi_2$. For a unit vector $\psi \in \mathcal{H}$, the corresponding density matrix is $\rho = |\psi\rangle\langle\psi|$.

Let $\{\varphi_j\}_{j=1}^d$ be an orthonormal basis of \mathcal{H} . (From now on, the term *basis* means an orthonormal basis.) If we perform a measurement of this basis in a state ρ , then we get an outcome j with the probability $\langle\varphi_j|\rho\varphi_j\rangle$. The probability distribution $p(j) = \langle\varphi_j|\rho\varphi_j\rangle$ encodes the information that this measurement gives us about the unknown state ρ . It is quite clear that this information is not enough to determine the input state uniquely. For instance, the pure states corresponding to the unit vectors $1/\sqrt{2}(\varphi_1 \pm \varphi_2)$ are different but they lead to the same probability distribution. If our aim is to identify an unknown quantum state uniquely, we should thus measure more than one orthonormal basis.

Let $\mathcal{B}_1 = \{\varphi_j^1\}_{j=1}^d, \dots, \mathcal{B}_m = \{\varphi_j^m\}_{j=1}^d$ be m orthonormal bases of \mathcal{H} . We say that the bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ distinguish two different states ρ_1 and ρ_2 if

$$\langle\varphi_j^\ell|\rho_1\varphi_j^\ell\rangle \neq \langle\varphi_j^\ell|\rho_2\varphi_j^\ell\rangle \quad (1)$$

for some $\ell = 1, \dots, m$ and $j = 1, \dots, d$. This means that if we get the probability distributions related to all m bases in the states ρ_1 and ρ_2 , then the measurement data corresponding to these two states are different.

We say that the orthonormal bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ *distinguish all pure states* if they distinguish any pair of different pure states. Following [12], we also say that in this case the bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ are *informationally complete with respect to pure states*.

We recall that it is possible to find finite collections of orthonormal bases that can distinguish all pure states. Namely, it is known that there exist $d + 1$ orthonormal bases which distinguish *all* states, pure or mixed; see e.g. [13] for a construction. Less than $d + 1$ bases cannot distinguish all states simply because not enough parameters are determined. However, the pure states form a non-convex subset of all states, and one cannot thus rule out the possibility that less than $d + 1$ bases can distinguish all pure states. This leads to our main question stated in the title:

How many orthonormal bases are needed in order to distinguish all pure states?

One may be tempted to criticize this question on the grounds that in any real experiment the states are perhaps never completely pure. But as any problem of this type, also this should be considered as a question on the fundamental limits of quantum theory. As such, we believe that it reveals an interesting and even surprising aspect of the duality of states and measurements.

3 Qubit and insufficiency of two bases

As a warm up, let us consider the case of a qubit, i.e., $d = 2$. It is well known and explained also in almost any textbook that one can choose three orthonormal bases such that the related measurement outcome distributions determine an unknown qubit state uniquely. This is rather obvious if one looks at the Bloch representation $\rho_{\vec{r}} = \frac{1}{2}(\mathbb{1} + \vec{r} \cdot \vec{\sigma})$ of qubit states, where \vec{r} is a vector in \mathbb{R}^3 satisfying $\|\vec{r}\| \leq 1$ and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ consists of Pauli matrices. Since

$$\vec{r} = (\text{tr}[\rho\sigma_x], \text{tr}[\rho\sigma_y], \text{tr}[\rho\sigma_z]),$$

we conclude that measurements of the eigenbases of σ_x , σ_y and σ_z specify the vector \vec{r} and hence also the state $\rho_{\vec{r}}$. More generally, if we fix three linearly independent unit vectors \vec{a} , \vec{b} and \vec{c} in \mathbb{R}^3 , then the measurements of the eigenbases of $\vec{a} \cdot \vec{\sigma}$, $\vec{b} \cdot \vec{\sigma}$ and $\vec{c} \cdot \vec{\sigma}$ distinguish all states.

A qubit state $\rho_{\vec{r}}$ is pure exactly when $\|\vec{r}\| = 1$. The direction of a unit vector \vec{r} depends on two parameters only, so one may wonder if two orthonormal bases can suffice to determine any pure qubit state. This is not true, in fact, in any dimension:

Proposition 1. *In any dimension $d \geq 2$, two orthonormal bases cannot distinguish all pure states.*

Proof. Our proof of this statement has been motivated by Theorem 1 in reference [14]. Let $\mathcal{B}_1 = \{\varphi_j\}_{j=1}^d$ and $\mathcal{B}_2 = \{\phi_k\}_{k=1}^d$ be two orthonormal bases of a d -dimensional Hilbert space. We need to find two nonparallel unit vectors ψ_+ and ψ_- such that

$$|\langle\xi|\psi_+\rangle|^2 = |\langle\xi|\psi_-\rangle|^2 \quad (2)$$

for all vectors $\xi \in \mathcal{B}_1 \cup \mathcal{B}_2$.

Let $\eta \in \mathcal{H}$ be a unit vector orthogonal to φ_1 . We set $\psi_{\pm} = \frac{1}{\sqrt{2}}(\varphi_1 \pm \eta)$. Then

$$|\langle \psi_{\pm} | \xi \rangle|^2 = \frac{1}{2} \left(|\langle \varphi_1 | \xi \rangle|^2 + |\langle \eta | \xi \rangle|^2 \right) \pm \operatorname{Re} (\langle \varphi_1 | \xi \rangle \langle \xi | \eta \rangle),$$

so that

$$|\langle \psi_+ | \xi \rangle|^2 - |\langle \psi_- | \xi \rangle|^2 = 2 \operatorname{Re} (\langle \varphi_1 | \xi \rangle \langle \xi | \eta \rangle).$$

Since $\langle \varphi_1 | \varphi_j \rangle \langle \varphi_j | \eta \rangle = 0$ for all $\varphi_j \in \mathcal{B}_1$, the condition (2) holds for all $\xi \in \mathcal{B}_1 \cup \mathcal{B}_2$ if

$$\operatorname{Re} (\langle \varphi_1 | \phi_k \rangle \langle \phi_k | \eta \rangle) = 0 \quad (3)$$

for all $\phi_k \in \mathcal{B}_2$. The remaining thing is to show that it is possible to choose a unit vector $\eta \in \mathcal{H}$ such that η is orthogonal to φ_1 and (3) holds for all $\phi_k \in \mathcal{B}_2$.

Firstly, suppose that $\langle \varphi_1 | \phi_1 \rangle = 0$ or $\langle \varphi_1 | \phi_2 \rangle = 0$. Then the corresponding choice $\eta = \phi_1$ or $\eta = \phi_2$ implies that (3) holds for all $\phi_k \in \mathcal{B}_2$. If otherwise $\langle \varphi_1 | \phi_1 \rangle \neq 0$ and $\langle \varphi_1 | \phi_2 \rangle \neq 0$, we then set

$$\eta = \frac{i |\langle \varphi_1 | \phi_1 \rangle \langle \varphi_1 | \phi_2 \rangle|}{\sqrt{|\langle \varphi_1 | \phi_1 \rangle|^2 + |\langle \varphi_1 | \phi_2 \rangle|^2}} \times (\langle \varphi_1 | \phi_1 \rangle^{-1} \phi_1 - \langle \varphi_1 | \phi_2 \rangle^{-1} \phi_2).$$

It is easy to verify that η is orthogonal to φ_1 . Furthermore, we get $\langle \varphi_1 | \phi_1 \rangle \langle \phi_1 | \eta \rangle = -\langle \varphi_1 | \phi_2 \rangle \langle \phi_2 | \eta \rangle = \frac{i |\langle \varphi_1 | \phi_1 \rangle \langle \varphi_1 | \phi_2 \rangle|}{\sqrt{|\langle \varphi_1 | \phi_1 \rangle|^2 + |\langle \varphi_1 | \phi_2 \rangle|^2}}$ and $\langle \varphi_1 | \phi_k \rangle \langle \phi_k | \eta \rangle = 0$ for $k \geq 3$, hence (3) holds for all $\phi_k \in \mathcal{B}_2$. \square

4 Rank criterion and qutrit

Let $\mathcal{B}_1 = \{\varphi_j^1\}_{j=1}^d, \dots, \mathcal{B}_m = \{\varphi_j^m\}_{j=1}^d$ be m orthonormal bases of \mathcal{H} . For each vector φ_j^ℓ , we denote $P_j^\ell = |\varphi_j^\ell\rangle\langle\varphi_j^\ell|$. Each P_j^ℓ is thus a 1-dimensional projection. Using this notation we observe that the orthonormal bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ cannot distinguish two different states ϱ_1 and ϱ_2 if and only if

$$\operatorname{tr} [P_j^\ell (\varrho_1 - \varrho_2)] = 0 \quad \text{for all } \ell = 1, \dots, m \text{ and } j = 1, \dots, d. \quad (4)$$

This condition means that the operator $\varrho_1 - \varrho_2$ is orthogonal to all the projections P_j^ℓ in the Hilbert-Schmidt inner product. (We recall that the Hilbert-Schmidt inner product of two operators A and B is $\langle A | B \rangle_{HS} = \operatorname{tr} [A^* B]$). Note that the operator $\varrho_1 - \varrho_2$ is selfadjoint and traceless. Moreover, if ϱ_1 and ϱ_2 are pure states, then $\varrho_1 - \varrho_2$ has rank 2.

The previous observation can be developed into a useful criterion when we look at all selfadjoint operators that are orthogonal to the projections P_j^ℓ . Suppose T is a nonzero selfadjoint operator satisfying

$$\operatorname{tr} [P_j^\ell T] = 0 \quad \text{for all } \ell = 1, \dots, m \text{ and } j = 1, \dots, d.$$

First of all, as $\sum_j P_j^\ell = \mathbb{1}$, the operator T satisfies $\operatorname{tr} [T] = 0$. To derive some other properties of T , we write T in the spectral decomposition

$$T = \sum_{i=1}^p \lambda_i^+ |\psi_i^+\rangle\langle\psi_i^+| - \sum_{i=1}^n \lambda_i^- |\psi_i^-\rangle\langle\psi_i^-|,$$

where $\lambda_1^+, \dots, \lambda_p^+$ and $-\lambda_1^-, \dots, -\lambda_n^-$ are the strictly positive and strictly negative eigenvalues of T , respectively, and $\psi_1^+, \dots, \psi_p^+, \psi_1^-, \dots, \psi_n^-$ are orthogonal unit vectors. From $\operatorname{tr} [T] = 0$ it follows that

$$\sum_{i=1}^p \lambda_i^+ = \sum_{i=1}^n \lambda_i^- \equiv \lambda.$$

The rank of T is $p + n$, the number of its nonzero eigenvalues counted with their multiplicities. As $T \neq 0$ and $\operatorname{tr} [T] = 0$, T must have both positive and negative eigenvalues, meaning that $n \geq 1$ and $p \geq 1$. Therefore, the rank of T is at least 2. If the rank of T is 2, then $n = p = 1$ and thus

$$\lambda^{-1} T = |\psi_1^+\rangle\langle\psi_1^+| - |\psi_1^-\rangle\langle\psi_1^-|.$$

This implies that the orthonormal bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ cannot distinguish the pure states $\varrho_1 = |\psi_1^+\rangle\langle\psi_1^+|$ and $\varrho_2 = |\psi_1^-\rangle\langle\psi_1^-|$.

Our previous discussion can be summarized in the form of the following criterion.

Proposition 2. *Orthonormal bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ can distinguish all pure states if and only if every nonzero selfadjoint operator T that satisfies*

$$\operatorname{tr} [P_j^\ell T] = 0 \quad \text{for all } \ell = 1, \dots, m \text{ and } j = 1, \dots, d \quad (5)$$

has rank at least 3.

Using this criterion we can prove the following statement.

Proposition 3. *In dimension $d = 3$,*

- (i) *three orthonormal bases cannot distinguish all pure states;*
- (ii) *four orthonormal bases can distinguish all pure states if and only if the Hilbert-Schmidt orthogonal complement of the projections $\{P_j^\ell \mid \ell = 1, 2, 3, 4, j = 1, 2, 3\}$ is either $\{0\}$ or is the linear span of a single invertible selfadjoint operator.*

Proof. Our proof is adapted from the analogous one of ([9], Prop. 5). By Proposition 2, m orthonormal bases $\mathcal{B}_1, \dots, \mathcal{B}_m$ in dimension $d = 3$ distinguish all pure states if and only if every nonzero selfadjoint operator $T \in \{P_j^\ell \mid \ell = 1, \dots, m, j = 1, 2, 3\}^\perp$ is invertible. We claim that in this case there cannot exist two linearly independent selfadjoint operators $T_1, T_2 \in \{P_j^\ell \mid \ell = 1, \dots, m, j = 1, 2, 3\}^\perp$.

Indeed, suppose on the contrary that T_1 and T_2 are two such operators. Since $\det(T_1)$ and $\det(T_2)$ are nonzero,

there are real numbers α_1, α_2 such that $\det(\alpha_1 T_1) > 0$ and $\det(\alpha_2 T_2) < 0$. By linear independence, the convex combination $\lambda \alpha_1 T_1 + (1 - \lambda) \alpha_2 T_2$ is nonzero for all $\lambda \in [0, 1]$. The determinant is a continuous function, and hence the intermediate value theorem implies that $\det[\lambda_0 \alpha_1 T_1 + (1 - \lambda_0) \alpha_2 T_2] = 0$ for some $\lambda_0 \in (0, 1)$. Therefore, the nonzero selfadjoint operator $T = \lambda_0 \alpha_1 T_1 + (1 - \lambda_0) \alpha_2 T_2$ is not invertible. But T satisfies (5), which then contradicts Proposition 2.

Now, observe that, if the linear space $\{P_j^\ell \mid \ell = 1, \dots, m, j = 1, 2, 3\}^\perp$ has dimension k , then we can find a basis of it consisting of selfadjoint operators. Indeed, if T_1, \dots, T_k is any linear basis, then the selfadjoint operators $T_1^+, \dots, T_k^+, T_1^-, \dots, T_k^-$ given by:

$$T_h^+ = T_h + T_h^*, \quad T_h^- = i(T_h - T_h^*)$$

still satisfy (5) and generate the linear space $\{P_j^\ell \mid \ell = 1, \dots, m, j = 1, 2, 3\}^\perp$. Extracting k linearly independent elements from these operators, we get the claimed basis of selfadjoint operators.

The proof of item (i) then follows by combining the previous two observations. Indeed, three orthonormal bases $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3$ give 9 projections P_j^ℓ . However, as $\sum_{j=1}^3 P_j^\ell = \mathbb{1}$ for each $\ell = 1, 2, 3$, at most 7 of them are linearly independent. The dimension of the linear space of all operators is 9, hence we conclude that $\dim\{P_j^\ell \mid \ell = 1, 2, 3, j = 1, 2, 3\}^\perp \geq 2$. Therefore, there are at least 2 linearly independent selfadjoint operators that are orthogonal to all projections P_j^ℓ , thus implying that $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3$ cannot distinguish all pure states.

In a similar way, four bases $\mathcal{B}_1, \dots, \mathcal{B}_4$ can distinguish all pure states only if the dimension of $\{P_j^\ell \mid \ell = 1, \dots, 4, j = 1, 2, 3\}^\perp$ is either $k = 0$ or $k = 1$. In the latter case, $\{P_j^\ell \mid \ell = 1, \dots, 4, j = 1, 2, 3\}^\perp = \mathbb{C}T$ for some selfadjoint operator T , which must then be invertible by Proposition 2. This proves the direct implication in item (ii). On the other hand, the converse statement is clear by Proposition 2. \square

In the next section, we will see that in dimension $d = 3$ there actually exist four orthonormal bases distinguishing all pure states. The condition in item (ii) of Proposition 3 is then very useful to explicitly construct such bases. As an example, Section 8 below will provide an application to the measurement of the orthonormal bases corresponding to four different spin directions in a spin-1 system.

5 Four bases that distinguish all pure states

Up to now we have seen that already in dimension 3, we can never find three orthonormal bases which would yield unique determination of all pure states. Therefore, the minimal number of bases in that case is at least four. In this section we show that, perhaps surprisingly, four properly chosen orthonormal bases are sufficient regardless of the dimension of the Hilbert space.

Proposition 4. *In any finite dimension, there exist four orthonormal bases $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3, \mathcal{B}_4$ that can distinguish all pure states.*

The proof is based on an explicit construction of the bases in the Hilbert space $\mathcal{H} = \mathbb{C}^d$, as presented by Jaming in [11]. His construction uses properties of the Hermite polynomials, but a similar construction works also for any other sequence of orthogonal polynomials. Different polynomials will lead to different bases, so this freedom in choosing the polynomials may be sometimes useful.

The construction begins by fixing a sequence of orthogonal polynomials. By a *sequence of orthogonal polynomials* we mean a sequence p_0, p_1, p_2, \dots of real polynomials such that the degree of p_n is n and

$$\int_a^b p_n(x) p_\ell(x) w(x) dx = \delta_{n\ell}$$

for a nonnegative weight function w and either finite or infinite interval $[a; b]$. The most common sequences of orthogonal polynomials are the (normalized versions of) Chebyshev, Hermite, Laguerre and Legendre polynomials. For instance, the n th Hermite polynomial H_n is defined by the formula

$$H_n(x) = \frac{(-1)^n}{\sqrt{2^n n!}} e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

The Hermite polynomials form a sequence of orthogonal polynomials with respect to the weight function $w(x) = \frac{1}{\sqrt{\pi}} e^{-x^2}$ and the infinite interval $(-\infty; \infty)$.

The following construction uses three basic properties shared by any sequence of orthogonal polynomials. Let c_n denote the highest coefficient of a polynomial p_n . It can be shown (see e.g. [15], pp. 43–46) that the following properties hold:

- (a) The roots of p_n are all real and distinct.
- (b) p_n and p_{n+1} have no common roots.
- (c) For all $x \neq y$, the *Christoffel-Darboux formula* holds:

$$\sum_{j=0}^n p_j(x) p_j(y) = \frac{c_n}{c_{n+1}} \frac{p_{n+1}(x) p_n(y) - p_n(x) p_{n+1}(y)}{x - y}.$$

In dimension d , only the first $d + 1$ polynomials of the sequence will be needed.

To construct the first basis, let x_1, \dots, x_d be the roots of the polynomial p_d , and define

$$\tilde{\varphi}_j^1 = (p_0(x_j), p_1(x_j), \dots, p_{d-1}(x_j))^T \quad (6)$$

for $j = 1, \dots, d$. Then each vector $\tilde{\varphi}_j^1$ is nonzero since $p_0(x_j) \neq 0$ (p_0 is a nonzero constant polynomial), and since the zeros are all distinct, we may apply the Christoffel-Darboux formula to get

$$\begin{aligned} \langle \tilde{\varphi}_i^1 | \tilde{\varphi}_j^1 \rangle &= \sum_{k=0}^{d-1} p_k(x_i) p_k(x_j) \\ &= \frac{c_{d-1}}{c_d} \frac{p_d(x_i) p_{d-1}(x_j) - p_{d-1}(x_i) p_d(x_j)}{x_i - x_j} = 0 \end{aligned}$$

for $i \neq j$. Thus, the vectors are orthogonal. By normalizing $\varphi_j^1 = \|\tilde{\varphi}_j^1\|^{-1}\tilde{\varphi}_j^1$ we obtain an orthonormal basis $\mathcal{B}_1 = \{\varphi_j^1\}_{j=1}^d$ of \mathbb{C}^d .

Let then y_1, \dots, y_{d-1} be the roots of the polynomial p_{d-1} and define

$$\tilde{\varphi}_j^2 = (p_0(y_j), p_1(y_j), \dots, p_{d-1}(y_j))^T, \quad (7)$$

for $j = 1, \dots, d-1$. These vectors are again nonzero and orthogonal, and since the y_j 's are the roots of p_{d-1} , the last component is $p_{d-1}(y_j) = 0$. Hence, we can again normalize $\varphi_j^2 = \|\tilde{\varphi}_j^2\|^{-1}\tilde{\varphi}_j^2$ and define $\varphi_d^2 = (0, \dots, 0, 1)^T$ to obtain another orthonormal basis $\mathcal{B}_2 = \{\varphi_j^2\}_{j=1}^d$.

For the two remaining bases, we first pick a number $\alpha \in \mathbb{R}$ which is not a rational multiple of π . We then define

$$\tilde{\varphi}_j^3 = (p_0(x_j), e^{i\alpha}p_1(x_j), \dots, e^{i(d-1)\alpha}p_{d-1}(x_j))^T, \quad (8)$$

which, after normalization, gives the third basis $\mathcal{B}_3 = \{\varphi_j^3\}_{j=1}^d$. Finally, we set

$$\tilde{\varphi}_j^4 = (p_0(y_j), e^{i\alpha}p_1(y_j), \dots, e^{i(d-1)\alpha}p_{d-1}(y_j))^T \quad (9)$$

which, after normalizing and adding the vector $\varphi_d^4 = (0, \dots, 0, 1)^T$, gives the last basis $\mathcal{B}_4 = \{\varphi_j^4\}_{j=1}^d$.

Using the basis $\mathcal{B}_1, \dots, \mathcal{B}_4$, we can now prove our main result.

Proof of Proposition 4. As usual, we denote $P_j^\ell = |\varphi_j^\ell\rangle\langle\varphi_j^\ell|$ for $\ell = 1, \dots, 4$ and $j = 1, \dots, d$. By (4), in order to prove that the bases $\mathcal{B}_1, \dots, \mathcal{B}_4$ can distinguish all pure states, we need to show that, for any two pure states $\varrho_1 = |\xi\rangle\langle\xi|$ and $\varrho_2 = |\eta\rangle\langle\eta|$, the condition

$$\text{tr}[P_j^\ell(\varrho_1 - \varrho_2)] = 0 \quad \text{for all } \ell = 1, \dots, 4 \text{ and } j = 1, \dots, d \quad (10)$$

implies $\xi = e^{i\theta}\eta$ for some $\theta \in \mathbb{R}$. To see this, let $T = \varrho_1 - \varrho_2$, and write $T = (t_{ij})_{i,j=1}^d$ with respect to the standard basis of \mathbb{C}^d . The selfadjointness of T implies that $t_{ii} \in \mathbb{R}$ and $t_{ji} = \overline{t_{ij}}$. Using the explicit form of the vectors from (6)–(9), the orthogonality condition (10) then yields

$$\sum_{k,l=0}^{d-1} t_{k+1,l+1} p_k(z)p_l(z) = 0 \quad (11)$$

$$\sum_{k,l=0}^{d-1} t_{k+1,l+1} e^{i(l-k)\alpha} p_k(z)p_l(z) = 0 \quad (12)$$

for every $z \in \{x_1, \dots, x_d, y_1, \dots, y_{d-1}\}$. The degree of p_n is n , so the polynomials in (11) and (12) have degree at most $2d-2$. But the above equations state that these polynomials have $2d-1$ distinct roots, so they are actually identically zero. Therefore, (11) and (12) hold for all $z \in \mathbb{R}$.

We can now look at the highest order terms in (11) and (12). This corresponds to $k = l = d-1$ so that by linear independence of the monomials $1, z, z^2, \dots, z^{2d-2}$ we have $t_{d,d} = 0$. Since

$$t_{ij} = \xi_i \overline{\xi_j} - \eta_i \overline{\eta_j} \quad \text{for all } i, j,$$

it follows that $|\xi_d|^2 = |\eta_d|^2$ so that $\xi_d = e^{i\theta}\eta_d$ for some $\theta \in \mathbb{R}$. Assume for the moment that $\xi_d \neq 0$.

We can now consider the terms of order $2d-3$. Since they appear only for $k = d-1$ and $l = d-2$ or vice versa, we must have

$$t_{d,d-1} + t_{d-1,d} = t_{d,d-1}e^{-i\alpha} + t_{d-1,d}e^{i\alpha} = 0.$$

By substituting $t_{d-1,d} = \overline{t_{d,d-1}}$ we then get

$$\text{Re}(t_{d,d-1}) = \text{Re}(t_{d,d-1}e^{-i\alpha}) = 0.$$

Since $e^{-i\alpha} \notin \mathbb{R}$, we have $t_{d,d-1} = 0$ which implies that $\xi_d \overline{\xi_{d-1}} = \eta_d \overline{\eta_{d-1}}$. By our assumption, $\xi_{d-1} = e^{i\theta}\eta_{d-1}$.

We now proceed by induction. Suppose that $\xi_{d-p} = e^{i\theta}\eta_{d-p}$ for $p = 0, \dots, n-1$. It follows that $t_{d-p,d-q} = 0$ for $p, q \leq n-1$, so that the highest order terms in (11) and (12) are of order $2d-n-2$, and they appear only with $k = d-1$ and $l = d-n-1$ or vice versa. This gives us

$$\text{Re}(t_{d,d-n}) = \text{Re}(t_{d,d-n}e^{-i\alpha}) = 0$$

so that $t_{d,d-n} = 0$. Hence, $\xi_{d-n} = e^{i\theta}\eta_{d-n}$.

Finally, if we have $\xi_d = 0$ so that also $\eta_d = 0$, then $t_{d,n} = 0$ and $t_{n,d} = 0$ for all n , and the summations in (11) and (12) terminate at $d-2$. Hence, we can repeat the above process starting from the highest order term which is now of order $2d-4$. By induction, if $\xi_d = \dots = \xi_{d-(n-1)} = 0$ but $\xi_{d-n} \neq 0$, then also $\eta_d = \dots = \eta_{d-(n-1)} = 0$ so that the process can be started from the terms of order $2(d-n)-2$ which would give $\xi_{d-n} = e^{i\theta}\eta_{d-n}$ and then proceed as before. This completes the proof of Proposition 4. \square

6 Insufficiency of three bases in dimension 5 and higher

We have seen that in every finite dimension $d = 2, 3, \dots$, it is possible to choose a set of four orthonormal bases that distinguish all pure states, but no pair of orthonormal bases can have this property. Can a set of three orthonormal bases distinguish all pure states? As we know already, this question has a positive answer in $d = 2$ and a negative answer in $d = 3$. In the following, we explain how topological considerations lead to a negative answer for all dimensions $d \geq 5$. For more details on the topological aspects of state determination we refer to [9,16].

First, it is useful to generalize the property of distinguishing pure states to arbitrary sets $\mathcal{A} = \{A_1, \dots, A_n\}$ of selfadjoint operators on \mathcal{H} . We say that such a set \mathcal{A} *distinguishes all pure states* if for two different pure states ϱ_1 and ϱ_2 , there exists $A_i \in \mathcal{A}$ such that

$$\text{tr}[A_i\varrho_1] \neq \text{tr}[A_i\varrho_2]. \quad (13)$$

Clearly, if \mathcal{A} consists of the orthogonal projections defined by a collection of orthonormal bases, we obtain again (1).

In what follows, we use the notation below: for each dimension $d = 2, 3, \dots$, we denote by:

- \mathfrak{s}_d the minimal number of *selfadjoint operators* which distinguish all pure states;
- \mathfrak{b}_d the minimal number of *orthonormal bases* which distinguish all pure states.

It is easy to see that \mathfrak{s}_d gives a lower bound for \mathfrak{b}_d . Namely, if we have m bases, they give $m \cdot d$ projections. All the projections corresponding to a basis sum up to the identity operator $\mathbb{1}$; since $\text{tr}[\mathbb{1}\varrho] = 1$ for all states ϱ , one projection for each basis can be left out without losing any information. We thus conclude that

$$(d-1) \cdot \mathfrak{b}_d \geq \mathfrak{s}_d. \quad (14)$$

Therefore, lower bounds for \mathfrak{s}_d translate into lower bounds for \mathfrak{b}_d .

Let us denote by \mathcal{P} the set of pure states. Saying that \mathcal{A} distinguishes all pure states means that the map

$$f^{\mathcal{A}}: \mathcal{P} \rightarrow \mathbb{R}^n, \quad \varrho \mapsto (\text{tr}[A_1\varrho], \dots, \text{tr}[A_n\varrho]) \quad (15)$$

is injective. Hence, roughly speaking, the selfadjoint operators \mathcal{A} distinguish all pure states if and only if the map (15) identifies \mathcal{P} with a subset of the Euclidean space \mathbb{R}^n . This is a very useful observation: suppose, for instance, that it is possible to prove that there is a natural number n_0 such that no injective map $\mathcal{P} \rightarrow \mathbb{R}^n$ exists if $n < n_0$; then one can conclude that $\mathfrak{s}_d \geq n_0$.

Up to this point our considerations were purely set theoretical. However, it can be proved that, if the map $f^{\mathcal{A}}$ is injective, then it is actually a smooth embedding (see Prop. 7 of Appendix A; we refer to [17] for the necessary notions from differential geometry). Therefore, the selfadjoint operators \mathcal{A} can distinguish all pure states only if the manifold of pure states \mathcal{P} can be smoothly embedded in \mathbb{R}^n .

The minimal n for which \mathcal{P} can be smoothly embedded in \mathbb{R}^n , is called the *embedding dimension* of \mathcal{P} . From the heuristic point of view, if M_1 and M_2 are two smooth manifolds of the same dimension, we expect that the embedding dimension of M_1 is greater than the embedding dimension of M_2 if the shape of M_1 is more involved than the shape of M_2 . For instance, a 2-dimensional torus can be smoothly embedded in \mathbb{R}^3 whereas the Klein bottle requires \mathbb{R}^4 .

The problem of determining the embedding dimension of complex projective spaces has been studied extensively in the mathematical literature and the best bounds are, up to our knowledge, those obtained in [18]. They lead to the conclusion that

$$\mathfrak{s}_d \geq \begin{cases} 4d - 2\alpha - 3 & \text{for all } d \geq 2 \\ 4d - 2\alpha - 2 & \text{for } d \text{ odd, and } \alpha \equiv 2 \pmod{4} \\ 4d - 2\alpha - 1 & \text{for } d \text{ odd, and } \alpha \equiv 3 \pmod{4} \end{cases} \quad (16)$$

where α is the number of 1's in the binary expansion of $d-1$ (see [9], Thm. 6).

Writing the expansion $d-1 = \sum_{j=0}^n a_j 2^j$, we have that $2^n \leq d-1$ if and only if $n \leq \log_2(d-1)$. Hence,

$$\alpha \leq n + 1 \leq \log_2(d-1) + 1,$$

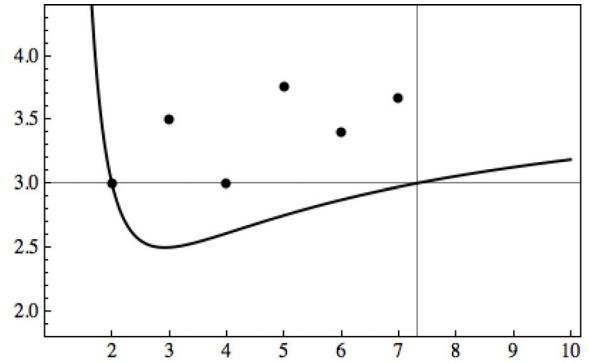


Fig. 1. The function $f(x) = 4 - \frac{2 \log_2(x-1) + 1}{x-1}$ gives a lower bound for the minimal number of orthonormal bases. Since $\mathfrak{b}_d \geq f(d)$, we conclude that $\mathfrak{b}_d \geq 4$ for all $d \geq 8$. For the dimensions $2 \leq d \leq 7$ we obtain a lower bound from Table 1. The dots correspond to $\mathfrak{s}_d/(d-1)$, which is a lower bound for \mathfrak{b}_d by (14).

Table 1.

d	\mathfrak{s}_d	$\mathfrak{s}_d/(d-1)$
2	3	3
3	7	3.5
4	9	3
5	15	3.75
6	17	3.4
7	22	3.67

so that

$$\mathfrak{s}_d \geq 4d - 2\alpha - 3 \geq 4d - 2 \log_2(d-1) - 5$$

for all $d \geq 2$. Inserting this into (14) we obtain

$$\mathfrak{b}_d \geq \frac{4d - 2 \log_2(d-1) - 5}{d-1} = 4 - \frac{2 \log_2(d-1) + 1}{d-1}. \quad (17)$$

To see the consequences of the derived lower bound (17), we examine the function

$$f: [2, \infty) \rightarrow \mathbb{R}, \quad f(x) = 4 - \frac{2 \log_2(x-1) + 1}{x-1}$$

(see Fig. 1). Firstly, we notice that $f(2) = 3$ and $\lim_{x \rightarrow \infty} f(x) = 4$. Secondly, the derivative $f'(x)$ has a single zero at $x_0 = 1 + \frac{e}{\sqrt{2}} \simeq 2.922$, and it satisfies $f'(x) < 0$ for $x \in (2, x_0)$ and $f'(x) > 0$ for $x > x_0$. Finally, $f(8) \simeq 3.055$ so that $f(x) > 3$ for all $x \geq 8$. Since \mathfrak{b}_d is an integer and $\mathfrak{b}_d \geq f(d)$, we thus have $\mathfrak{b}_d \geq 4$ for all $d \geq 8$.

For the dimensions $d = 2, \dots, 7$ we need to analyse the lower bound more carefully. In Table 1 we have calculated the values of the lower bound for \mathfrak{s}_d given in (16). We thus observe that unless $d = 2$ or 4 , three orthonormal bases cannot be sufficient.

In conclusion, for the dimensions $d = 3$ and $d \geq 5$ the minimal number of bases is four. For $d = 2$ the minimal number is three and in the case $d = 4$ it is, based on our knowledge, either three or four.

7 Insufficiency of four product bases in dimension $d = 4$

In our search for the minimal number of orthonormal bases that can distinguish all pure states, the remaining question is:

Is it possible to find three orthonormal bases in dimension 4 that can distinguish all pure states?

Unfortunately, we are able to provide only a partial answer to this question. Namely, in the following we will see that if we consider the splitting of the 4-dimensional Hilbert space into a tensor product $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$, then for any three bases consisting solely of product vectors, the answer is negative. In fact, we will show that even four product bases are not enough.

Before we concentrate on dimension 4, we slightly elaborate the state distinction criterion used in earlier sections. As we have seen, a set $\mathcal{A} = \{A_1, \dots, A_n\}$ of selfadjoint operators cannot distinguish between two states ϱ_1 and ϱ_2 if and only if

$$\text{tr}[A_j(\varrho_1 - \varrho_2)] = 0 \quad \text{for all } j = 1, \dots, n.$$

Since the trace is a linear functional, this is equivalent to

$$\text{tr} \left[\left(\sum_{j=1}^n \alpha_j A_j \right) (\varrho_1 - \varrho_2) \right] = 0 \quad \text{for all } \alpha_1, \dots, \alpha_n \in \mathbb{C}.$$

Moreover, as $\text{tr}[\varrho_1 - \varrho_2] = 0$, we can rewrite the previous condition as

$$\text{tr} \left[\left(\alpha_0 \mathbb{1} + \sum_{j=1}^n \alpha_j A_j \right) (\varrho_1 - \varrho_2) \right] = 0$$

for all $\alpha_0, \alpha_1, \dots, \alpha_n \in \mathbb{C}$.

This equivalent formulation shows that, for the purpose of state distinction, we can always switch from \mathcal{A} to the linear space spanned by \mathcal{A} and $\mathbb{1}$. We denote this subspace of operators by $\mathcal{R}(\mathcal{A})$, i.e.,

$$\mathcal{R}(\mathcal{A}) = \left\{ \alpha_0 \mathbb{1} + \sum_{j=1}^n \alpha_j A_j \mid \alpha_j \in \mathbb{C} \right\} \quad (18)$$

and call it the (complex) *operator system* generated by the selfadjoint operators \mathcal{A} . If the set \mathcal{A} consists of the projections corresponding to m orthonormal bases $\mathcal{B}_1 = \{\varphi_j^1\}_{j=1}^d, \dots, \mathcal{B}_m = \{\varphi_j^m\}_{j=1}^d$, we write also

$$\mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_m) = \mathcal{R}(\{P_j^\ell \mid \ell = 1, \dots, m, j = 1, \dots, d\}),$$

where as usual $P_j^\ell = |\varphi_j^\ell\rangle\langle\varphi_j^\ell|$. Our discussion then yields the following conclusion.

Proposition 5. *Let \mathcal{A} and \mathcal{A}' be two sets of selfadjoint operators. If $\mathcal{R}(\mathcal{A}) = \mathcal{R}(\mathcal{A}')$, then \mathcal{A} and \mathcal{A}' distinguish the same pairs of states.*

Let us make use of this fact to show that in the Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ four product bases cannot distinguish all pure states. By product basis, we mean an orthonormal basis of \mathcal{H} that is constructed from two orthonormal bases of \mathbb{C}^2 by taking their tensor product. More precisely, if $\{\varphi_1, \varphi_2\}$ and $\{\phi_1, \phi_2\}$ are two orthonormal bases of \mathbb{C}^2 , then $\{\varphi_i \otimes \phi_j \mid i, j = 1, 2\}$ is an orthonormal basis of \mathbb{C}^4 . From the physics point of view this corresponds to a scheme where two parties try to determine the unknown pure state of a composite system by performing only local measurements.

Using the Bloch representation, any 1-dimensional projection on \mathbb{C}^2 can be written as $P_{\vec{n}} = \frac{1}{2}(\mathbb{1} + \vec{n} \cdot \vec{\sigma})$, where $\vec{n} \in \mathbb{R}^3$ is a unit vector. Furthermore,

$$\text{tr}[P_{\vec{m}} P_{\vec{n}}] = \frac{1}{2}(1 + \vec{m} \cdot \vec{n}).$$

Therefore, the 1-dimensional projections corresponding to an orthonormal basis of \mathbb{C}^2 are $P_{\vec{n}}$ and $P_{-\vec{n}}$ where \vec{n} is fixed by the choice of the basis.

Suppose that we have two quadruples of (not necessarily distinct) orthonormal bases $\mathcal{B}'_1, \dots, \mathcal{B}'_4$ and $\mathcal{B}''_1, \dots, \mathcal{B}''_4$ of \mathbb{C}^2 with the corresponding quadruples of unit vectors $\vec{m}_1, \dots, \vec{m}_4$ and $\vec{n}_1, \dots, \vec{n}_4$. We define four product bases of \mathbb{C}^4 via

$$\mathcal{B}_j = \{\varphi \otimes \phi \mid \varphi \in \mathcal{B}'_j, \phi \in \mathcal{B}''_j\}.$$

The four projections

$$P_{\vec{m}_j} \otimes P_{\vec{n}_j}, \quad P_{\vec{m}_j} \otimes P_{-\vec{n}_j}, \quad P_{-\vec{m}_j} \otimes P_{\vec{n}_j}, \quad P_{-\vec{m}_j} \otimes P_{-\vec{n}_j}$$

corresponding to an orthonormal basis \mathcal{B}_j have the same linear span as the selfadjoint operators

$$\mathbb{1} \otimes \mathbb{1}, \quad \vec{m}_j \cdot \vec{\sigma} \otimes \mathbb{1}, \quad \mathbb{1} \otimes \vec{n}_j \cdot \vec{\sigma}, \quad \vec{m}_j \cdot \vec{\sigma} \otimes \vec{n}_j \cdot \vec{\sigma}.$$

Therefore, by introducing the set

$$\mathcal{A} = \{\vec{m}_j \cdot \vec{\sigma} \otimes \mathbb{1}, \mathbb{1} \otimes \vec{n}_j \cdot \vec{\sigma}, \vec{m}_j \cdot \vec{\sigma} \otimes \vec{n}_j \cdot \vec{\sigma} \mid j = 1, \dots, 4\},$$

we have the equality

$$\mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4) = \mathcal{R}(\mathcal{A}).$$

We will next show that there exist two maximally entangled pure states $\varrho_1 \neq \varrho_2$ which are not distinguished by the set \mathcal{A} , thus implying by Proposition 5 that the bases $\mathcal{B}_1, \dots, \mathcal{B}_4$ cannot distinguish all pure states.

Recall that a unit vector $\Omega \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is called *maximally entangled* if $\Omega = \frac{1}{\sqrt{2}}(\varphi_1 \otimes \phi_1 + \varphi_2 \otimes \phi_2)$ for some orthonormal bases $\{\varphi_1, \varphi_2\}$ and $\{\phi_1, \phi_2\}$ of \mathbb{C}^2 . If $\{e_1, e_2\}$ denotes the canonical basis of \mathbb{C}^2 , and $\Omega_0 = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 + e_2 \otimes e_2)$, then there always exists a unitary operator U on \mathbb{C}^2 such that $\Omega = (U \otimes \mathbb{1})\Omega_0$ (see, e.g., [19], Lem. 2). Since the global phase of Ω is irrelevant for our purposes, we see that the maximally entangled pure states are in one-to-one correspondence with elements of the quotient group $SU(2)/\{\pm I\}$, which in turn is diffeomorphic to $SO(3)$ through mapping $U \mapsto R_U$ given by the equality

$$U^* \vec{x} \cdot \vec{\sigma} U = R_U \vec{x} \cdot \vec{\sigma} \quad \text{for all } \vec{x} \in \mathbb{R}^3.$$

Suppose that we try to determine the pure state $\varrho_U = |\Omega\rangle\langle\Omega|$ using the selfadjoint operators \mathcal{A} . Since

$$\begin{aligned}\mathrm{tr}[(\vec{m}_j \cdot \vec{\sigma} \otimes \mathbb{1})\varrho_U] &= \mathrm{tr}[(U^* \vec{m}_j \cdot \vec{\sigma} U \otimes \mathbb{1})|\Omega_0\rangle\langle\Omega_0|] \\ &= \frac{1}{2}\mathrm{tr}[U^* \vec{m}_j \cdot \vec{\sigma} U] = 0\end{aligned}$$

and similarly

$$\begin{aligned}\mathrm{tr}[(\mathbb{1} \otimes \vec{n}_j \cdot \vec{\sigma})\varrho_U] &= \mathrm{tr}[(\mathbb{1} \otimes \vec{n}_j \cdot \vec{\sigma})|\Omega_0\rangle\langle\Omega_0|] \\ &= \frac{1}{2}\mathrm{tr}[\vec{n}_j \cdot \vec{\sigma}] = 0,\end{aligned}$$

we find that the only relevant information that can be extracted is

$$\begin{aligned}\mathrm{tr}[(\vec{m}_j \cdot \vec{\sigma} \otimes \vec{n}_j \cdot \vec{\sigma})\varrho_U] &= \mathrm{tr}[(U^* \vec{m}_j \cdot \vec{\sigma} U \otimes \vec{n}_j \cdot \vec{\sigma})|\Omega_0\rangle\langle\Omega_0|] \\ &= \mathrm{tr}[(R_U \vec{m}_j \cdot \vec{\sigma} \otimes \vec{n}_j \cdot \vec{\sigma})|\Omega_0\rangle\langle\Omega_0|] \\ &= h_j(R_U),\end{aligned}$$

where h_j is defined on the linear space $M_3(\mathbb{R})$ of real 3×3 matrices and is given by:

$$h_j(A) = \mathrm{tr}[(A \vec{m}_j \cdot \vec{\sigma} \otimes \vec{n}_j \cdot \vec{\sigma})|\Omega_0\rangle\langle\Omega_0|].$$

If the selfadjoint operators \mathcal{A} could distinguish all pure states, then, in particular, they could distinguish all maximally entangled pure states. Therefore, the linear map $f : M_3(\mathbb{R}) \rightarrow \mathbb{R}^4$ given by

$$f(A) = (h_1(A), h_2(A), h_3(A), h_4(A))^T$$

would restrict to an injective map $\tilde{f} : SO(3) \rightarrow \mathbb{R}^4$. By Proposition 8 in Appendix A, such a map would then be a smooth embedding of $SO(3)$ into \mathbb{R}^4 . Since $SO(3)$ is diffeomorphic to the real projective 3-dimensional space RP^3 by [20], Proposition 5.2.10, and RP^3 cannot be embedded into \mathbb{R}^4 by [21, 22], we then obtain a contradiction. We thus conclude that the selfadjoint operators \mathcal{A} cannot distinguish all pure states.

8 Spin-1 – It is not only about number of bases

As we have now seen, it is enough to measure four bases in order to distinguish all pure states. However, not all sets of four bases do this as was implied by our consideration of product bases in dimension 4. In this section we demonstrate this further by giving another example where some natural candidates for the bases fail to distinguish all pure states. We consider the problem of determining all pure states of a spin-1 system by measuring four orthonormal bases corresponding to different spin directions.

The Hilbert space of the spin-1 quantum system is $\mathcal{H} = \mathbb{C}^3$, and the usual spin operators along the three axes are

$$\begin{aligned}L_x &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, & L_y &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \\ L_z &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.\end{aligned}$$

If $\vec{n} \in \mathbb{R}^3$ is any unit vector, the spin operator along the direction \vec{n} is $\vec{n} \cdot \vec{L} = n_x L_x + n_y L_y + n_z L_z$, which is self-adjoint and has eigenvalues $\{+1, 0, -1\}$. We denote the corresponding eigenprojections as $P_j^{\vec{n}}$, and they can be written as:

$$\begin{aligned}P_{+1}^{\vec{n}} &= \frac{(\vec{n} \cdot \vec{L})^2 + \vec{n} \cdot \vec{L}}{2} & P_{-1}^{\vec{n}} &= \frac{(\vec{n} \cdot \vec{L})^2 - \vec{n} \cdot \vec{L}}{2} \\ P_0^{\vec{n}} &= \mathbb{1} - (\vec{n} \cdot \vec{L})^2.\end{aligned}$$

Note that these projections span the same linear space as the selfadjoint operators $\mathbb{1}$, $\vec{n} \cdot \vec{L}$, and $(\vec{n} \cdot \vec{L})^2$.

The next result shows that, if the four directions $\vec{n}_1, \dots, \vec{n}_4$ are suitably chosen, then the corresponding spin measurements actually determine all pure states. This refines the lower bound of [23], where the authors prove that all pure states of a spin-1 system are uniquely determined by six spin components, and should be compared with [24, 25], where it is shown that, for any spin- s system, the spin observables along two infinitesimally near directions \vec{n} and \vec{n}' together with the expectation value of the spin observable orthogonal to \vec{n} and \vec{n}' are enough to determine all pure states up to a set of measure zero.

Proposition 6. *Let $\vec{n}_1, \dots, \vec{n}_4 \in \mathbb{R}^3$ be four directions with components $\vec{n}_k = (n_{kx}, n_{ky}, n_{kz})^T$, and denote by \mathcal{B}_k the eigenbases of the spin operator along \vec{n}_k for a spin-1 quantum system. Then the bases $\mathcal{B}_1, \dots, \mathcal{B}_4$ distinguish all pure states if and only if the following conditions hold:*

(a) *the 4×5 real matrix M with entries*

$$\begin{aligned}M_{k,1} &= 2\sqrt{2}n_{kx}n_{kz} & M_{k,2} &= -2\sqrt{2}n_{ky}n_{kz} \\ M_{k,3} &= n_{kx}^2 - n_{ky}^2 & M_{k,4} &= -2n_{kx}n_{ky} \\ M_{k,5} &= 3n_{kz}^2 - 1\end{aligned}\tag{19}$$

has rank 4;

(b) *there exists a nonzero real solution $x = (x_1, \dots, x_5)^T \in \mathbb{R}^5$ of the linear system $Mx = 0$ such that*

$$2x_1x_2x_4 + x_3(x_1^2 - x_2^2) + x_5(x_1^2 + x_2^2 + x_5^2 - x_3^2 - x_4^2) \neq 0.\tag{20}$$

Proof. We will show that conditions (a) and (b) in the previous statement are equivalent to the condition in item (ii) of Proposition 3.

The operator system $\mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)$ is spanned by $\mathbb{1}$ and the set of 8 selfadjoint operators

$$\mathcal{A} = \{\vec{n}_1 \cdot \vec{L}, \dots, \vec{n}_4 \cdot \vec{L}, (\vec{n}_1 \cdot \vec{L})^2, \dots, (\vec{n}_4 \cdot \vec{L})^2\}.$$

Since the operators $\{\vec{n}_1 \cdot \vec{L}, \dots, \vec{n}_4 \cdot \vec{L}\}$ are linearly dependent, we have $\dim \mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4) \leq 8$, that is, $\dim \mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)^\perp \geq 1$. Hence by Proposition 3.(ii) we actually need to show that conditions (a) and (b) are equivalent to

(a') $\dim \mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)^\perp = 1$;

(b') there exists an invertible selfadjoint operator $T \in \mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)^\perp$.

We begin by showing that conditions (a) and (a') are equivalent, and, when (a) holds

$$\mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)^\perp = \Phi(\ker(M)), \quad (21)$$

where $\Phi: \mathbb{C}^5 \rightarrow M_3(\mathbb{C})$ is the linear map given by:

$$\Phi \begin{pmatrix} x_1 \\ \vdots \\ x_5 \end{pmatrix} = \begin{pmatrix} x_5 & x_1 + ix_2 & x_3 + ix_4 \\ x_1 - ix_2 & -2x_5 & -x_1 - ix_2 \\ x_3 - ix_4 & -x_1 + ix_2 & x_5 \end{pmatrix}.$$

Note that Φ is injective, and $\Phi(\mathbb{C}^5) = \{\mathbb{1}, L_x, L_y, L_z\}^\perp$. Moreover, it is easy to check that $\text{tr}[(\vec{n}_i \cdot \vec{L})^2 \Phi(x)] = m_i x$ for all $x \in \mathbb{C}^5$, where m_i is the i th row of the matrix M defined in (19), and $m_i x$ is the usual matrix product. Hence,

$$\begin{aligned} \Phi(\ker(M)) &= \{\mathbb{1}, L_x, L_y, L_z\}^\perp \cap \{(\vec{n}_1 \cdot \vec{L})^2, \dots, (\vec{n}_4 \cdot \vec{L})^2\}^\perp \\ &= \mathcal{R}(\mathcal{A}')^\perp \end{aligned} \quad (22)$$

where

$$\mathcal{A}' = \{L_x, L_y, L_z, (\vec{n}_1 \cdot \vec{L})^2, \dots, (\vec{n}_4 \cdot \vec{L})^2\}.$$

Now, suppose that $\text{rank}(M) < 4$. Then, $\dim \ker(M) > 1$, from which it follows that $\dim \mathcal{R}(\mathcal{A}')^\perp > 1$ by injectivity of Φ . Since $\mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4) = \mathcal{R}(\mathcal{A})$ and $\mathcal{A} \subset \mathcal{A}'$, we have $\mathcal{R}(\mathcal{A}')^\perp \subset \mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)^\perp$, and this implies that condition (a') does not hold.

Conversely, assume that $\text{rank}(M) = 4$. We claim that in this case the four unit vectors $\vec{n}_1, \dots, \vec{n}_4$ span the whole space \mathbb{R}^3 . Indeed, if e.g. $\vec{n}_i = \alpha_i \vec{n}_1 + \beta_i \vec{n}_2$ for $i = 3, 4$, then we would have

$$(\vec{n}_i \cdot \vec{L})^2 = \alpha_i^2 (\vec{n}_1 \cdot \vec{L})^2 + \beta_i^2 (\vec{n}_2 \cdot \vec{L})^2 + \alpha_i \beta_i \{ \vec{n}_1 \cdot \vec{L}, \vec{n}_2 \cdot \vec{L} \},$$

where $\{\cdot, \cdot\}$ is the anticommutator. Hence, $m_i = \alpha_i^2 m_1 + \beta_i^2 m_2 + \alpha_i \beta_i u$, where $u^T \in \mathbb{C}^5$ (actually, $u^T \in \mathbb{R}^5$) is defined by:

$$u x = \text{tr} \left[\left\{ \vec{n}_1 \cdot \vec{L}, \vec{n}_2 \cdot \vec{L} \right\} \Phi(x) \right]$$

for all $x \in \mathbb{C}^5$. Thus, $\text{rank}(M) \leq 3$, which is a contradiction. Our claim then implies $\mathcal{R}(\mathcal{A}) = \mathcal{R}(\mathcal{A}')$. Taking the orthogonal complement, we have $\mathcal{R}(\mathcal{A})^\perp = \mathcal{R}(\mathcal{A}')^\perp = \Phi(\ker(M))$ by (22), and (21) follows since $\mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4) = \mathcal{R}(\mathcal{A})$. In particular, by injectivity of Φ , $\dim \mathcal{R}(\mathcal{B}_1, \dots, \mathcal{B}_4)^\perp = \dim \ker(M) = 1$, that is, condition (a').

Finally, assuming (a), we come to the proof of (b) \Leftrightarrow (b'). First of all, observe that the operator $\Phi(x)$ is selfadjoint if and only if $x \in \mathbb{R}^5$. By (21), condition (b') then amounts to

$$\det \begin{pmatrix} x_5 & x_1 + ix_2 & x_3 + ix_4 \\ x_1 - ix_2 & -2x_5 & -x_1 - ix_2 \\ x_3 - ix_4 & -x_1 + ix_2 & x_5 \end{pmatrix} \neq 0$$

for some nonzero $x = (x_1, \dots, x_5)^T \in \mathbb{R}^5$ such that $Mx = 0$, that is, condition (b). \square

By Proposition 6, it is easy to check that the three orthogonal spin directions \vec{e}_1, \vec{e}_2 , and \vec{e}_3 cannot be completed to a set of four directions which would allow unique determination of pure states. Indeed, if $\vec{n}_1 = \vec{e}_1, \vec{n}_2 = \vec{e}_2, \vec{n}_3 = \vec{e}_3$ and \vec{n}_4 is any direction, then

$$\text{rank}(M) = \text{rank} \begin{pmatrix} 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 2 \\ * & * & * & * & * \end{pmatrix} \leq 3$$

thus contradicting condition (a).

However, there exist sets of four spin directions which distinguish all pure states. For example, it is easy to check that the unit vectors

$$\begin{aligned} \vec{n}_1 &= (0, 0, 1)^T & \vec{n}_2 &= (1/\sqrt{2}, 1/\sqrt{2}, 0)^T \\ \vec{n}_3 &= (1/\sqrt{2}, 0, 1/\sqrt{2})^T & \vec{n}_4 &= (0, \sqrt{3}/2, 1/2)^T \end{aligned}$$

satisfy both conditions (a) and (b) of Proposition 6, hence the corresponding bases can distinguish all pure states.

Finally, we remark that the property of distinguishing all pure states is robust against small perturbations of the unit vectors $\vec{n}_1, \dots, \vec{n}_4$. Indeed, suppose that conditions (a) and (b) of Proposition 6 are satisfied by the four directions $\vec{n}_1^0, \dots, \vec{n}_4^0$. The matrix $M = M(\vec{n}_1, \dots, \vec{n}_4)$ defined in (19) is a continuous function of $(\vec{n}_1, \dots, \vec{n}_4)$, hence so are the diagonalizable matrix-valued functions M^*M and MM^* . By condition (a), the 4×4 matrix $MM^*(\vec{n}_1^0, \dots, \vec{n}_4^0)$ is invertible, hence MM^* is invertible in a neighborhood of $(\vec{n}_1^0, \dots, \vec{n}_4^0)$, that is, $\text{rank}(M) = 4$ in that neighborhood. Thus, condition (a) still holds around $(\vec{n}_1^0, \dots, \vec{n}_4^0)$. Now, let $x \in \mathbb{R}^5$ be a nonzero real solution of $M(\vec{n}_1^0, \dots, \vec{n}_4^0)x = 0$ which satisfies (20). Moreover, let Q be the orthogonal projection onto $\ker(M^*M)$, and define $\tilde{x}(\vec{n}_1, \dots, \vec{n}_4) = Q(\vec{n}_1, \dots, \vec{n}_4)x$. By [26], Theorem II.5.1, Q is a continuous function of $(\vec{n}_1, \dots, \vec{n}_4)$ in a neighborhood of $(\vec{n}_1^0, \dots, \vec{n}_4^0)$. As M^*M is a real matrix, also Q is real. Combining these two facts, the map \tilde{x} is a nonzero continuous \mathbb{R}^5 -valued function such that $\tilde{x} \in \ker(M^*M) = \ker(M)$ and $\tilde{x}(\vec{n}_1^0, \dots, \vec{n}_4^0) = x$. By continuity, \tilde{x} satisfies (20) around $(\vec{n}_1^0, \dots, \vec{n}_4^0)$. Therefore, also condition (b) of Proposition 6 remains fulfilled for small perturbations of $(\vec{n}_1^0, \dots, \vec{n}_4^0)$. We conclude that, if the eigenbases of the spin operators along the directions $\vec{n}_1^0, \dots, \vec{n}_4^0$ distinguish all pure states, then this still holds true in a neighborhood of these directions.

9 Remarks on the question in infinite dimensional Hilbert space

The question of the title is meaningful also in the case of an infinite dimensional Hilbert space. The proof of Proposition 1 works without changes also in that case, so we conclude that two orthonormal bases cannot distinguish all pure states even when $d = \infty$. However, the construction of four orthonormal bases in Section 5 has no direct generalization to the infinite dimensional Hilbert space.

We are, in fact, not aware of a construction in infinite dimension that would give a finite number of bases that can distinguish all pure states.

In the infinite dimensional case it is natural to allow also measurements of continuous observables such as position Q and momentum P . In fact, the determination of pure states from the statistics of such measurements was precisely what was addressed in the original Pauli problem. Since it is known that Q and P alone are not sufficient for this purpose, we can ask if this set can be suitably completed to make it able to distinguish all pure states. One natural attempt to obtain such a completion would be to add rotated quadratures $Q_\theta = \cos \theta Q + \sin \theta P$. It is known that by measuring all of the quadratures, it is possible to determine an arbitrary state, pure or mixed [27], but it is not known if a smaller subset is sufficient for pure state determination. It was recently shown that no triple $\{Q_{\theta_1}, Q_{\theta_2}, Q_{\theta_3}\}$ of quadratures is enough [28]. In particular, it is not sufficient to measure position, momentum, and a single additional rotated quadrature.

For larger, but still finite, sets of rotated quadratures it is only known that if such a set can distinguish all pure states, then the choice of the angles θ is a delicate issue. In [28], it was shown that if a finite set of angles $\theta_1, \dots, \theta_n$ satisfies $\theta_i - \theta_j \in \mathbb{Q}\pi$ for all $i, j = 1, \dots, n$, then the corresponding observables are not sufficient for pure state determination. In [29], a similar result was proved in the case that $\cot \theta_j \in \mathbb{Q}$ for all $j = 1, \dots, n$.

JS and AT acknowledge financial support from the Italian Ministry of Education, University and Research (FIRB project RBFR10COAQ).

Appendix A: Linear smooth embeddings in \mathbb{R}^n

If M is a real differentiable manifold and $x \in M$, we denote by $T_x(M)$ the (real) tangent space of M at x . If N is another differentiable manifold and $f : M \rightarrow N$ is a differentiable map, we let $df_x : T_x(M) \rightarrow T_{f(x)}(N)$ be the differential of f at x .

In this section we assume that M is a submanifold of a real linear space V , and we prove that, if a linear map $f : V \rightarrow \mathbb{R}^n$ restricts to an injective map $\tilde{f} : M \rightarrow \mathbb{R}^n$, then \tilde{f} is a smooth embedding in the following two cases:

1. $V = S_d(\mathbb{C})$ is the linear space of complex $d \times d$ selfadjoint matrices and $M = \mathcal{P}$ is the submanifold of pure states (see [9], Sect. 4.2);
2. $V = M_3(\mathbb{R})$ is the linear space of real 3×3 matrices and $M = SO(3)$ is the submanifold of orthogonal matrices with unit determinant.

The next two results are Theorem 5 and a particular case of Lemma 1 in [9]. Up to our knowledge, Proposition 8 below is new.

Lemma 1. *Let V, W be two real linear spaces, and M a compact submanifold of V . Suppose that $T_x(M) \subseteq \mathbb{R}(M - M)$ for all $x \in M$. Then, if a linear map $f : V \rightarrow W$*

restricts to an injective map $\tilde{f} : M \rightarrow W$, the restriction \tilde{f} is a smooth embedding of M in V .

Proof. Since M is compact and \tilde{f} is continuous, injectivity implies that \tilde{f} is a homeomorphism of M onto $\tilde{f}(M)$ [30], Proposition 1.6.8. In order to show that it is a smooth embedding, it remains to prove that $d\tilde{f}_x$ is injective for all $x \in M$.

Note that by the linearity of f $d\tilde{f}_x = f|_{T_x(M)}$ for all $x \in M$. Thus, if $u \in T_x(M)$ with $u = \lambda(x_1 - x_2)$ for some $\lambda \in \mathbb{R}$ and $x_1, x_2 \in M$, then

$$d\tilde{f}_x u = f(u) = \lambda(f(x_1) - f(x_2)) = \lambda(\tilde{f}(x_1) - \tilde{f}(x_2)) \equiv 0$$

if and only if $\lambda = 0$ or $\tilde{f}(x_1) = \tilde{f}(x_2)$, that is, $x_1 = x_2$ by injectivity of \tilde{f} . In both cases, we have $u = 0$, hence $d\tilde{f}_x$ is injective as claimed. \square

Proposition 7. *If $\tilde{f} : \mathcal{P} \rightarrow \mathbb{R}^n$ is injective and it is the restriction of a linear map $f : S_d(\mathbb{C}) \rightarrow \mathbb{R}^n$, then \tilde{f} is a smooth embedding of \mathcal{P} in \mathbb{R}^n .*

Proof. By Lemma 1, it suffices to prove that $T_\varrho(\mathcal{P}) \subseteq \mathbb{R}(\mathcal{P} - \mathcal{P})$ for all pure states $\varrho \in \mathcal{P}$. Indeed, \mathcal{P} is an orbit for the adjoint action of the group $SU(d)$ on the linear space $S_d(\mathbb{C})$, hence

$$\begin{aligned} T_\varrho(\mathcal{P}) &= \left\{ \frac{d}{dt} e^{itH} \varrho e^{-itH} \mid H \in S_d(\mathbb{C}) \right\} \\ &= \{i[H, \varrho] \mid H \in S_d(\mathbb{C})\}. \end{aligned}$$

If ϱ is a pure state and $H \in S_d(\mathbb{C})$, then $i[H, \varrho]$ is a self-adjoint traceless matrix with rank at most 2. Therefore, $i[H, \varrho] = \lambda(|\psi^+\rangle\langle\psi^+| - |\psi^-\rangle\langle\psi^-|)$ for some $\lambda \in \mathbb{R}$ and unit vectors $\psi^+, \psi^- \in \mathbb{C}^d$, which proves the claim. \square

Proposition 8. *If $\tilde{f} : SO(3) \rightarrow \mathbb{R}^n$ is injective and it is the restriction of a linear map $f : M_3(\mathbb{R}) \rightarrow \mathbb{R}^n$, then \tilde{f} is a smooth embedding of $SO(3)$ in \mathbb{R}^n .*

Proof. Again, by Lemma 1 it is enough to prove that $T_R(SO(3)) \subseteq \mathbb{R}(SO(3) - SO(3))$ for all $R \in SO(3)$.

Denote by $M_3^-(\mathbb{R})$ the linear subspace of antisymmetric matrices in $M_3(\mathbb{R})$. Then, $T_R(SO(3)) = RM_3^-(\mathbb{R})$ for all $R \in SO(3)$, so that it suffices to show that any $X \in M_3^-(\mathbb{R})$ can be written $X = \lambda(R_0 - R_0^T)$ for some $R_0 \in SO(3)$ and $\lambda \in \mathbb{R}$. Indeed, the map $g : SO(3) \rightarrow M_3^-(\mathbb{R})$ with $g(R) = R - R^T$ is a diffeomorphism of an open neighborhood U of the identity I onto a neighborhood $g(U)$ of 0, since its differential

$$dg_I(X) = \frac{d}{dt} (\exp(tX) - \exp(-tX)) \Big|_{t=0} = 2X$$

is bijective. It follows that $\mathbb{R}g(U) = M_3^-(\mathbb{R})$, hence the claim.

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