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Mitsuru Hamada

Quantum ICT Research Institute, Tamagawa University
6-1-1 Tamagawa-gakuen, Machida, Tokyo 194-8610, Japan

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Mitsuru Hamada
Quantum Information Science Research Center
Quantum ICT Research Institute
Tamagawa University
6-1-1 Tamagawa-gakuen, Machida, Tokyo 194-8610, Japan

***Abstract*—A conversion between two parameterizations for SU(2) is presented. One parameterization is well-known and it is in terms of a triple of rotation angles called Euler angles, and the other generalizes this parameterization. The latter is involved similarly with a triple of angles for rotation while the configuration of the three axes for rotation is the most general possible.**

I. Introduction

Motivated by some problems on quantum computation, the author has recently investigated issues on rotations in the Euclidean space and the corresponding unitary operations. Specifically, in a recent article [1], the author presented a concrete expression for the minimum number of rotations required for constructing an arbitrarily given target rotation (under some constraint), and more importantly, an algorithm for giving an optimal, i.e., minimum-achieving construction. The present article extracts a result related to parameterizations of rotations from [1]. It is on a conversion between two parameterizations for SU(2) in terms of triples of rotation angles. Among the two parameterizations, one is well-known and it is in terms of Euler angles [2], and the other generalizes this parameterization.

The reasons for presenting this result include (i) that the result seems useful for treating other issues for its generality, (ii) that the conversion was not fully but only partially presented in [1], (iii) that explicitly showing a region of parameters that makes the generalized parameterization *one-to-one* (Remark 2) will be useful in view of the fact that even in the special case of the classical parameterization with Euler angles [2], many authors have not paid enough attention to this issue, which has led to propagation of an error in the literature, and (iv) that this result may serve, especially for non-specialists, as an introduction to the issue treated in [1]. In fact, the main result in [1] could not have been obtained without the result to be presented below (and a lemma already reported in a previous article of this author [3][1]).

II. Definitions

Let X, Y and Z denote the Pauli matrices:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Throughout, I denotes the 2×2 identity matrix. The transpose of a vector $\hat{v}$ is denoted by $\hat{v}^{\mathrm{T}}$.

We put

$$R_{\hat{v}}(\theta) = (\cos\tfrac{\theta}{2})I - i(\sin\tfrac{\theta}{2})(v_x X + v_y Y + v_z Z), \quad (1)$$

where $\hat{v} = (v_x, v_y, v_z)^{\mathrm{T}} \in \mathbb{R}^3$ with $\|\hat{v}\| = \sqrt{v_x^2 + v_y^2 + v_z^2} = 1$ and $\theta \in \mathbb{R}$, with $\mathbb{R}$ denoting the set of real numbers (e.g., [5]). This represents the rotation about $\hat{v}$ by angle θ (through the homomorphism in Section III-B). The matrices $R_y(\theta)$ and $R_z(\theta)$ denote the following special cases of $R_{\hat{v}}(\theta)$, respectively:

$$R_y(\theta) := R_{\hat{y}}(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix},$$

where

$$\hat{y} = (0, 1, 0)^{\mathrm{T}},$$

and

$$R_z(\theta) := R_{\hat{z}}(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix},$$

where

$$\hat{z} = (0, 0, 1)^{\mathrm{T}}.$$

We put $\mathrm{S}^2 = \{\hat{v} \in \mathbb{R}^3 \mid \|v\| = 1\}$. The set of 2×2 unitary matrices with determinant 1 and the set of 3×3 real orthogonal matrices with determinant 1 are denoted by SU(2) and SO(3), respectively. They stand for the special unitary group and the special orthogonal group, respectively.

III. Preliminaries

A. Standard Expressions for SU(2) Elements

In this section, standard parametric expressions of elements of SU(2) are reviewed. (Most expressions can be found in [2], [5] unless another source is specified.)

A-1. Expression with (a, b) and $R_{\hat{v}}(\theta)$: It is well-known and easy to check that any matrix in SU(2) can be written as

$$W(a, b) := \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \quad (2)$$

with some complex numbers a and b with $|a|^2 + |b|^2 = 1$ [2, Chapter 15], and hence, as

$$\begin{pmatrix} w + iz & y + ix \\ -y + ix & w - iz \end{pmatrix} = wI + i(xX + yY + zZ) \quad (3)$$

[1] Specifically, that lemma was in an unpublished manuscript, an abstract of which is [4]. Later, when this was used to give the constructive result in [1], it was reduced to a form neater than the original.

with some real numbers x, y, z and w with

$$w^2 + x^2 + y^2 + z^2 = 1. \tag{4}$$

From this expression of an arbitrary matrix in SU(2), we obtain another parameterization as follows.

Take a real number θ such that $\cos(\theta/2) = w$ and $\sin(\theta/2) = \sqrt{1-w^2} = \sqrt{x^2+y^2+z^2}$; write x, y and z as $x = -v_x \sin(\theta/2)$, $y = -v_y \sin(\theta/2)$ and $z = -v_z \sin(\theta/2)$, where $v_x, v_y, v_z \in \mathbb{R}$ and $v_x^2 + v_y^2 + v_z^2 = 1$. Thus, using real numbers $\theta, v_x, v_y, v_z \in \mathbb{R}$ with $v_x^2 + v_y^2 + v_z^2 = 1$, any matrix in SU(2) can be written (e.g., [5]) as

$$(\cos \tfrac{\theta}{2}) I - i(\sin \tfrac{\theta}{2})(v_x X + v_y Y + v_z Z),$$

which is nothing but $R_{\hat{v}}(\theta)$ in (1).

In (1), using spherical coordinates for parameterizing $\hat{v} \in \mathrm{S}^2$, we have a parameterization of SU(2) as in [3, Section III]. That expression was derived there from the requirement that $R_{\hat{v}}(\theta)$ act as a rotation on $\mathbb{R}^3$.[2]

A-2. Expression with Euler angles $R_y(\alpha)R_z(\beta)R_y(\gamma)$: Rewriting (2) or by a direct calculation, we obtain the following expression of an SU(2) element. Any matrix in SU(2) can be written as

$$\begin{pmatrix} e^{-i\eta} \cos \frac{\beta}{2} & -e^{i\zeta} \sin \frac{\beta}{2} \\ e^{-i\zeta} \sin \frac{\beta}{2} & e^{i\eta} \cos \frac{\beta}{2} \end{pmatrix} \tag{5}$$

and hence, as

$$\begin{pmatrix} e^{-i\frac{\gamma+\alpha}{2}} \cos \frac{\beta}{2} & -e^{i\frac{\gamma-\alpha}{2}} \sin \frac{\beta}{2} \\ e^{-i\frac{\gamma-\alpha}{2}} \sin \frac{\beta}{2} & e^{i\frac{\gamma+\alpha}{2}} \cos \frac{\beta}{2} \end{pmatrix}, \tag{6}$$

where $\eta, \zeta, \alpha, \beta$ and γ are real numbers. This is another parameterization for SU(2). Note the above matrix in (6) equals $R_z(\alpha)R_y(\beta)R_z(\gamma)$. The parameters α, β and γ are known as Euler angles.

B. Homomorphism from SU(2) onto SO(3)

The reader, if unfamiliar with the topic, may wonder in what sense SU(2) is related to rotations in the three-dimensional Euclidean space. This will be explained in this section.

For $U \in \mathrm{SU}(2)$, we denote by $F(U)$ the matrix of the linear transformation on $\mathbb{R}^3$ that sends $(x, y, z)^{\mathrm{T}}$ to $(x', y', z')^{\mathrm{T}}$ through[3]

$$U(xX + yY + zZ)U^\dagger = x'X + y'Y + z'Z. \tag{7}$$

Namely, for any $(x, y, z)^{\mathrm{T}}, (x', y', z')^{\mathrm{T}} \in \mathbb{R}^3$ with (7),

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = F(U) \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

[2]That parameterization in [3] does not seem standard. Mentioning this, although it is not used in what follows, is for the following reason. In one widely accepted definition, parameters ought to be independent variables. The one in [3] is a parameterization in this strong sense. Still, (1) and (2) are useful 'parametric' expressions.

[3]Note that in defining the homomorphism in [2], Wigner has used $-Y$ and $-Z$ in place of our Y and Z, which causes a slight difference between his homomorphism and ours, that is, F.

We also define

$$\hat{R}_{\hat{v}}(\theta) := F\big(R_{\hat{v}}(\theta)\big), \quad \hat{v} \in \mathrm{S}^2, \theta \in \mathbb{R}. \tag{8}$$

Example. We have

$$\hat{R}_y(\theta) := F(R_y(\theta)) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \tag{9}$$

and

$$\hat{R}_z(\theta) := F(R_z(\theta)) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{10}$$

□

Thus, $\hat{R}_y(\theta)$ and $\hat{R}_z(\theta)$ represent rotations. It can be seen that $R_{\hat{v}}(\theta)$ with the general $\hat{v} \in \mathrm{S}^2$ also represents a rotation (see, e.g., [5] or [3, Section III]).

IV. Regions of Parameters for Expressing the Whole SU(2)

In this section, we will remark that the choice of (α, β, γ) for expressing any given matrix in SU(2) is unique if we restrict the region of (α, β, γ) appropriately. Specifically, we define the following.

Definition 1: For $S, T, S_0, T_0 \in \mathbb{R}$,

$$\begin{aligned} A_{S,T} &:= \{(\alpha, \beta, \gamma) \mid 0 < \beta < \pi,\ S \le \gamma + \alpha < S + 4\pi, \\ &\qquad T \le \gamma - \alpha < T + 4\pi\}, \\ B_{S,T_0} &:= \{(\alpha, 0, \gamma) \mid S \le \gamma + \alpha < S + 4\pi,\ \gamma - \alpha = T_0\}, \\ C_{S_0,T} &:= \{(\alpha, \pi, \gamma) \mid \gamma + \alpha = S_0,\ T \le \gamma - \alpha < T + 4\pi\} \end{aligned}$$

and

$$D_{S,T;S_0,T_0} := A_{S,T} \cup B_{S,T_0} \cup C_{S_0,T}.$$

A typical choice for the constants S, T, S_0, T_0 would be $T = S = -2\pi$ (or $= 0$) and $T_0 = S_0 = 0$.

Example.

$$\begin{aligned} A_{-2\pi,-2\pi} &:= \{(\alpha, \beta, \gamma) \mid 0 < \beta < \pi,\ -\pi \le \tfrac{\gamma+\alpha}{2} < \pi, \\ &\qquad -\pi \le \tfrac{\gamma-\alpha}{2} < \pi\}, \\ B_{-2\pi,0} &:= \{(\alpha, 0, \gamma) \mid -\pi \le \tfrac{\gamma+\alpha}{2} < \pi,\ \gamma - \alpha = 0\} \end{aligned}$$

and

$$C_{0,-2\pi} = \{(\alpha, \pi, \gamma) \mid \gamma + \alpha = 0,\ -\pi \le \tfrac{\gamma-\alpha}{2} < \pi\}.$$

□

Definition 2: A function $V : \mathbb{R}^3 \to \mathrm{SU}(2)$ is defined by

$$V(\alpha, \beta, \gamma) = \begin{pmatrix} e^{-i\frac{\gamma+\alpha}{2}} \cos \frac{\beta}{2} & -e^{i\frac{\gamma-\alpha}{2}} \sin \frac{\beta}{2} \\ e^{-i\frac{\gamma-\alpha}{2}} \sin \frac{\beta}{2} & e^{i\frac{\gamma+\alpha}{2}} \cos \frac{\beta}{2} \end{pmatrix}.$$

As usual, the restriction of a function $g : D \to C$ to B, where $B \subset D$, is denoted by $g|_B$, which is the function $g|_B : B \to C$ such that $g(x) = g|_B(x)$ for $x \in B$. Then, the mapping $V|_D :\ D \to \mathrm{SU}(2)$, where $D = D_{S,T;S_0,T_0}$, is a bijection. Namely, we have the following.

Fact 1: For any $S, T, S_0, T_0 \in \mathbb{R}$, the function $V|_D : D \to \mathrm{SU}(2)$, where $D = D_{S,T;S_0,T_0}$, is one-to-one and $V|_D(D) = \mathrm{SU}(2)$.

This is easy from the mathematical viewpoint. Therefore, the author thought it unnecessary for those working in any fields that indispensably need mathematics when he first wrote this as a personal memorandum. However, he recently learned that many famous textbooks on quantum physics contained an error, which could have been avoided if the authors of these had considered the matter carefully to notice the above fact (see Section VI).

In view of this history, we shall mention that this fact is easy to see using the transformation between (α, γ) and (η, ζ) specified by

$$\eta = \frac{\gamma + \alpha}{2} \quad \text{and} \quad \zeta = \frac{\gamma - \alpha}{2}, \tag{11}$$

which has been used for rewriting (5) as (6). In fact, define the function $\tilde{V}(\beta, \eta, \zeta)$ such that $\tilde{V}(\beta, \eta, \zeta) = V|_D(\alpha, \beta, \gamma)$, where the domain of $\tilde{V}$ is the one transformed from $D = D_{S,T;S_0,T_0}$ with (11). Then, we see that $\tilde{V}$ is a bijection. This implies that the map $V|_D$ is also a bijection.

To sum up the above arguments, note the matrix in (6) equals $R_z(\alpha)R_y(\beta)R_z(\gamma)$. We have seen that any matrix in $\mathrm{SU}(2)$ can be decomposed into $R_z(\alpha)R_y(\beta)R_z(\gamma)$, $(\alpha, \beta, \gamma) \in D_{S,T;S_0,T_0}$, in a one-to-one manner.

V. Parameterizations with Triples of Angles

The material of this section up to Corollary 1, to be given, is from [1].

First, for a natural presentation of the result, we give a slightly more general form of the parameterization $R_z(\alpha)R_y(\beta)R_z(\gamma)$, replacing the y-axis and z-axis with a pair of orthogonal axes for rotation, as follows.

Lemma 1: Let $\hat{l}, \hat{m} \in \mathrm{S}^2$ be vectors with $\hat{l}^{\mathrm{T}}\hat{m} = 0$. Then, for any $U \in \mathrm{SU}(2)$, there exist some $\alpha, \gamma \in \mathbb{R}$ and $\beta \in [0, \pi]$ such that

$$U = R_{\hat{m}}(\alpha)R_{\hat{l}}(\beta)R_{\hat{m}}(\gamma). \tag{12}$$

If a proof is needed, see [1].

Now, we will present the conversion between two parameterizations through two lemmas and a corollary.

Lemma 2: [1]. Given any $\delta \in \mathbb{R}$ and $\hat{l}, \hat{m} \in \mathrm{S}^2$ such that $\hat{l}^{\mathrm{T}}\hat{m} = 0$, put

$$\hat{n} = (\sin\delta)\hat{l} \times \hat{m} + (\cos\delta)\hat{m}. \tag{13}$$

For an arbitrary $U \in \mathrm{SU}(2)$, choose parameters $\alpha', \beta', \gamma' \in \mathbb{R}$ such that

$$R_{\hat{l}}(-\delta)U = R_{\hat{m}}(\alpha')R_{\hat{l}}(\beta')R_{\hat{m}}(\gamma'). \tag{14}$$

Then,

$$U = R_{\hat{n}}(\alpha')R_{\hat{l}}(\beta' + \delta)R_{\hat{m}}(\gamma'). \tag{15}$$

Remark 1: Conversely, under the assumption (13), if U satisfies (15) for parameters $\alpha', \beta', \gamma' \in \mathbb{R}$, then (14) holds.

Remark 2: In the lemma, restricting $(\alpha', \beta', \gamma')$ to $D_{S,T;S_0,T_0}$, $S, T, S_0, T_0 \in \mathbb{R}$, as in Section IV, we see (15) gives a one-to-one parameterization of $\mathrm{SU}(2)$.

Corollary 1: [1]. Besides the premise of Lemma 2, assume $\beta' \in [0, \pi]$ and $U = R_{\hat{m}}(\alpha)R_{\hat{l}}(\beta)R_{\hat{m}}(\gamma)$ for some $\alpha, \beta, \gamma \in \mathbb{R}$. Then, β' is given as $\beta' = f(\alpha, \beta, \delta)$, where the function $f : \mathbb{R}^3 \to [0, \pi]$ is defined by

$$f(\alpha, \beta, \delta) := 2\arccos\Big[\cos^2\tfrac{\beta}{2}\cos^2\tfrac{\delta}{2} + \sin^2\tfrac{\beta}{2}\sin^2\tfrac{\delta}{2} + 2\cos\alpha\sin\tfrac{\beta}{2}\sin\tfrac{\delta}{2}\cos\tfrac{\beta}{2}\cos\tfrac{\delta}{2}\Big]^{\frac{1}{2}}.$$

Proof. Note $R_{\hat{l}}(\delta)R_{\hat{m}}(\alpha')R_{\hat{l}}(-\delta) = R_{\hat{n}}(\alpha')$, which is equivalent to $R_y(\delta)R_z(\alpha')R_y(-\delta) = R_v(\alpha')$, where $\hat{v} = (\sin\delta, 0, \cos\delta)^{\mathrm{T}}$ (see [1, Lemma 3.4] if one needs a proof; see also Fig. 1 therein), and therefore, can be checked easily by a direct calculation. Using this equation, we can rewrite (14) as $U = R_{\hat{n}}(\alpha')R_{\hat{l}}(\beta' + \delta)R_{\hat{m}}(\gamma')$, which is (15). This completes the proof of the lemma and Remark 1. The corollary follows from another direct calculation ([1, p. 10], or Lemma 3 below). □

The corollary can be obtained via the following lemma, where we use the expression with (a, b) in (2).

Lemma 3: Given any $\delta \in \mathbb{R}$ and $U \in \mathrm{SU}(2)$, let a, b be the complex numbers such that

$$R_y(-\delta)U = W(a, b). \tag{16}$$

If $U = R_z(\alpha)R_y(\beta)R_z(\gamma)$, where $\alpha, \beta, \gamma \in \mathbb{R}$, then,

$$\begin{aligned} a &= \cos\frac{\delta}{2}\cos\frac{\beta}{2}e^{-i\frac{\gamma+\alpha}{2}} + \sin\frac{\delta}{2}\sin\frac{\beta}{2}e^{-i\frac{\gamma-\alpha}{2}}, \\ b &= \sin\frac{\delta}{2}\cos\frac{\beta}{2}e^{i\frac{\gamma+\alpha}{2}} - \cos\frac{\delta}{2}\sin\frac{\beta}{2}e^{i\frac{\gamma-\alpha}{2}}. \end{aligned}$$

Proof. A short direct calculation shows the lemma. □

Note that β' in Corollary 1 is obtained as $\beta' = f(\alpha, \beta, \delta) = 2\arccos|a|$. The other parameters α' and γ' in Lemma 2, under the assumption $U = R_z(\alpha)R_y(\beta)R_z(\gamma)$, can be obtained similarly from a, b. Namely, α' and γ' are obtained as

$$\alpha' = -\arg(-b) - \arg a \quad \text{and} \quad \gamma' = \arg(-b) - \arg a, \tag{17}$$

respectively.[4]

Thus, we have elucidated a relation between the two parameterizations in

$$R_{\hat{z}}(\alpha)R_{\hat{y}}(\beta)R_{\hat{z}}(\gamma) = R_{\hat{v}}(\alpha')R_{\hat{y}}(\beta' + \delta)R_{\hat{z}}(\gamma'),$$

where $\hat{v} = (\sin\delta, 0, \cos\delta)^{\mathrm{T}}$, $\delta \in \mathbb{R}$, or a conversion from (α, β, γ) into $(\alpha', \beta', \gamma')$; the relation holds true if $\hat{y}$, $\hat{z}$ and $\hat{v}$ are replaced with $\hat{l}, \hat{m} \in \mathrm{S}^2$ and

$$\hat{n} = (\sin\delta)\hat{l} \times \hat{m} + (\cos\delta)\hat{m},$$

respectively, where $\hat{l}^{\mathrm{T}}\hat{m} = 0$.

[4]We follow the convention that the real number $\arg 0$ can be chosen arbitrarily. For $c \neq 0$, $\arg c$ is unique up to differences modulo 2π. If the complete uniqueness is preferred, one can use Fact 1.

VI. Discussions

Lemma 2 is a secondary part of Proposition 4.7 in [1]. A parameterization in the form $\hat{R}_{\hat{n}}(\alpha')\hat{R}_{\hat{l}}(\beta'')\hat{R}_{\hat{m}}(\gamma')$ for SO(3), where $\hat{l}$ is perpendicular to both $\hat{n}$ and $\hat{m}$ as in Lemma 2, has been known in the literature (see [6] for a history). One may wonder if a similar parameterization is possible when we remove the restriction on $\hat{n}, \hat{l}, \hat{m} \in \mathrm{S}^2$. This is impossible (unless we give up expressing the whole set of rotations). In fact, from [6, Theorem 3] (or by another way not presented here), it follows that the matrix $R_{\hat{n}}(\alpha')R_{\hat{l}}(\beta'')R_{\hat{m}}(\gamma')$ with the parameters $\alpha', \beta'', \gamma' \in \mathbb{R}$ exhausts the whole group SU(2) if and only if $\hat{l}$ is perpendicular to both $\hat{n}$ and $\hat{m}$.[5]

The relation among the parameters $\alpha, \beta, \gamma, \beta' \in \mathbb{R}$ in Lemma 2 and Corollary 1 was found by this author [1]. The present article supplements this result to give the relation among the whole parameters $\alpha, \beta, \gamma, \alpha', \beta', \gamma' \in \mathbb{R}$. (Note that the chief achievement of [1] is an algorithm for constructing a sequence of rotations of the minimum length that constitute an arbitrary target rotation; the full relation presented above was not pursued there.)

Advantages of Lemma 2 would be illustrated by its implications Remark 2, Corollary 1 and (17) as well as the constructive results of [1].

Regarding the error mentioned in Section IV, it is related to an orthogonality relation, which is fundamental in representation theory. This has been pointed out in [7], where they have presented what is denoted by $\overline{A_{0,-2\pi}}$ in the present article. As they pointed out, using this region for integration, we have a correct orthogonality relation while many authors misunderstood that a smaller region was enough for this purpose. Here, $\overline{A}$ denotes the closure of A. Now that we have Fact 1, we see that the correct orthogonality relation holds when we use $\overline{A_{S,T}}$ as the integration region for any $S, T \in \mathbb{R}$.

VII. Summary

A conversion between two parameterizations for SU(2) was presented. This conversion was, in part, already used in [1] in order to obtain a constructive optimal result, i.e., an algorithm for giving an optimal solution to an issue of constructing an arbitrary rotation.

Acknowledgments

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[5] They claimed essentially the same statement for SO(3) in place of SU(2). Note that the kernel of the homomorphism F is $\{I, -I\}$.

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