Geometry of projective unitary operators

If we identify unitary operators that have the same action on classes given by the projective equivalence, we get the *Projective Unitary Group*, which we denote by PU(2) (two denotes the dimension). We thereby identify the operator U with the operator $e^{i\varphi}U$. (Recall that $e^{i\varphi}$ here represents the so-called *scalar matrix*, i.e. a diagonal matrix with all indices on the diagonal equal to $e^{i\varphi}$, thus having the determinant $e^{i2\varphi}$.)

First, let us explore what the general unitary operator U looks like. Its first column is some unit vector $\begin{pmatrix} a \\ b \end{pmatrix}$. The second column is then perpendicular to it, so it is the vector $\begin{pmatrix} -b^* \\ a^* \end{pmatrix}$ up to multiplication by a complex unit. The general form of a unitary matrix is therefore

$$U = \begin{pmatrix} a & -e^{i\psi}b^* \\ b & e^{i\psi}a^* \end{pmatrix},$$

with determinant $e^{i\psi}$. In the basis of eigenvectors, the U is of the form

$$\begin{pmatrix} e^{i\varphi_1} & 0 \\ 0 & e^{i\varphi_2} \end{pmatrix},$$

where $\psi = \varphi_1 + \varphi_2$. The matrix U is projectively equivalent to the matrix

$$e^{-i\frac{\psi}{2}}U = \begin{pmatrix} e^{-i\psi/2}a & -e^{i\psi/2}b^* \\ e^{-i\psi/2}b & e^{i\psi/2}a^* \end{pmatrix} = \begin{pmatrix} c & -d^* \\ d & c^* \end{pmatrix},$$

where $c = e^{-i\psi/2}a$ and $d = e^{-i\psi/2}b$, with determinant one and the diagonal form

$$\begin{pmatrix} e^{-i\omega/2} & 0 \\ 0 & e^{i\omega/2} \end{pmatrix},$$

where $\omega = \varphi_2 - \varphi_1$. It is therefore natural to choose this simple representative of unitary operators projectively equivalent with U. It is an element of the *Special Unitary group* denoted SU(2). However, there are two such representatives! Namely $\pm e^{-i\psi/2}U$.

> **Remark:** Another natural choice is the matrix $e^{-i\varphi_1}U$, with the diagonal form
>
> $$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\omega} \end{pmatrix}.$$
>
> Note an interesting difference. While the mapping
>
> $$R(\omega) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\omega} \end{pmatrix}$$
>
> has the period 2π, the mapping
>
> $$T(\omega) = \begin{pmatrix} e^{-i\frac{\omega}{2}} & 0 \\ 0 & e^{i\frac{\omega}{2}} \end{pmatrix}$$
>
> has the period 4π, and the matrices $T(\omega)$ and $T(\omega + 2\pi)$ differ by the sign, being two representatives of PU(2) in SU(2).

Writing $c = p - ti$ and $d = s - ri$, where $p, r, s, t \in \mathbb{R}$, $(p, r, s, t) \in \mathbb{S}^3$, we have

$$\begin{pmatrix} p - ti & -s - ri \\ s - ri & p + ti \end{pmatrix}.$$

The sign in SU(2) can now be chosen in order to make p non-negative. (If $p = 0$ we will decide according to t or even s.) The advantage of this expression is the equality

$$\begin{pmatrix} p - ti & -s - ri \\ s - ri & p + ti \end{pmatrix} = pE + r(-iX) + s(-iY) + t(-iZ),$$

which provides a decomposition into matrices E, $-iX$, iY, $-iZ$ which satisfy the defining relations of quaternion units $1, \ell, j, k$. We can therefore identify $\ell = -iX$, $j = -iY$, $k = -iZ$ and we obtain a one-to-one correspondence between unit quaternions with non-negative real part and PU(2). Every element $U \in \mathrm{PU}(2)$ can be uniquely expressed as

$$U = \cos\frac{\omega}{2} E + (x\ell + yj + zk)\sin\frac{\omega}{2},$$

where $(x, y, z) \in \mathbb{S}^2$ and $\omega \in [0, \pi]$. In quantum mechanics, this is often written using so called *extended Euler's formula*

$$U = e^{-i\frac{\omega}{2}\,\xi\cdot\sigma} = E\cos\frac{\omega}{2} - i\,\xi\cdot\sigma\sin\frac{\omega}{2} = \cos\frac{\omega}{2}E + (x\ell + yj + zk)\sin\frac{\omega}{2},$$

where $\xi = (x, y, z)$ a $\sigma = (X, Y, Z)$. Each pair ξ, ω defines the rotation $R(\xi, \omega)$ of $\mathbb{R}^3$ around the axis ξ by the angle ω. These rotations make the *Special Orthonormal group* SO(3), that is, the group of matrices whose columns (and rows) form an orthonormal basis, and their determinant is one. Each non-identity rotation is thereby defined by two pairs due to the equality $R(\xi, \omega) = R(-\xi, -\omega)$.

> **Remark:** Identity matrix E brings about some technical difficulties, since its "axis" can be chosen arbitrarily (and $\omega = 0$). It is natural to adopt the convention for E that $x = y = z = 0$, that is, $\xi = \vec{0}$.

Therefore we have a bijection between $\mathbb{S}^2 \times (0, 2\pi)$ and $\mathrm{SU}(2) \setminus \{E\}$, where always two elements correspond to a single rotation in SO(3), or in PU(2). The above considerations can be summarized as follows:

$$\mathrm{PU}(2) \cong \mathrm{SU}(2)/\mathbb{Z}_2 \cong \mathbb{S}^3/\mathbb{Z}_2 \cong \mathbb{K}_1/\mathbb{Z}_2 \cong \mathbb{S}^2 \times (0, 2\pi)/\mathbb{Z}_2 \cup (\vec{0}, 0) \cong \mathrm{SO}(3).$$

By $\cong$ we loosely mean the above described identifications.

The first and the last elements of the are nevertheless related in a much more precise way, which is given by the relation between rotations and quaternion conjugations formulated in the following theorem.

Věta. The mapping

$$\begin{aligned} \Phi : \mathrm{SO}(3) &\to \mathrm{PU}(2) \\ R(\xi, \omega) &\mapsto e^{-i\frac{\omega}{2}\,\xi\cdot\sigma} \end{aligned}$$

is a group isomorphism. Moreover, for each rotation $\rho \in \mathrm{SO}(3)$ we have

$$\rho = \mathcal{S}^{-1} \circ \Phi(\rho) \circ \mathcal{S},$$

where $\mathcal{S} : \mathbb{S}^2 \to \mathbb{C}\mathbf{P}^1$ is the stereographic projection.

Důkaz. For $U = e^{-i\frac{\omega}{2}\,\xi\cdot\sigma}$ we have

$$R(\xi,\omega) = \rho_U \overset{\Phi}{\longmapsto} U.$$

The mapping is therefore injective and surjective, and the composition of rotations corresponds to the matrix multiplication. It remains to show that $R(\xi,\omega)$ acts on $\mathcal{S}^{-1}(|\psi\rangle)$ in the same way as U on $|\psi\rangle$. Here we exploit the density operator. Operator of the image $U|\psi\rangle$ is of the form

$$U|\psi\rangle\langle\psi|U^\dagger = \frac{1}{2}E + \frac{i}{2}U(b\ell + cj + dk)U^\dagger\,.$$

From the theorem about the action of quaternion conjugation we deduce that $\mathcal{S}^{-1}\left(U|\psi\rangle\right)$ is indeed equal to $\rho_U(b,c,d)$. Hence the following diagram commutes.

$$\begin{array}{ccc} \mathbb{C}\mathbf{P}^1 & \xleftarrow{\ \mathcal{S}\ } & \mathbb{S}^2 \\ {\scriptstyle e^{-i\frac{\omega}{2}\,\xi\cdot\sigma}}\big\downarrow & & \big\downarrow{\scriptstyle R(\xi,\omega)} \\ \mathbb{C}\mathbf{P}^1 & \xleftarrow{\ \mathcal{S}\ } & \mathbb{S}^2 \end{array}$$

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