Lecture notes: Qubit representations and rotations

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I. WHAT IS A QUBIT?

Let us begin by introducing some notation:

1 state (called "minus" on the Bloch sphere)

$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{the alternate symbol is } |-\rangle$$

0 state (called "plus" on the Bloch sphere)

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{the alternate symbol is } |+\rangle.$$

When you learn about the Bloch sphere (discussed below) you will see why the alternate symbols $|+\rangle$ and $|-\rangle$ are used to denote logical states.[1]

So what is a qubit? A qubit is the fundamental quantum state representing the smallest unit of quantum information containing one bit of classical information accessible by measurement. We simply take a qubit to be a mathematical object (an abstraction of a two-state quantum object) with a "one" state and a "zero" state:

$$|q\rangle = \alpha|0\rangle + \beta|1\rangle = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{1}$$

where α and β are complex numbers. These complex numbers are called *amplitudes*. The basis states are orthonormal

$$\langle 0|0\rangle = \langle 1|1\rangle = 1 \tag{2a}$$
$$\langle 0|1\rangle = \langle 1|0\rangle = 0. \tag{2b}$$

In general, the qubit $|q\rangle$ in (1) is said to be in a superposition state of the two logical basis states $|0\rangle$ and $|1\rangle$. If α and β are complex, it would seem that a qubit should have four free real-valued parameters (two magnitudes and two phases):

$$|q\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \phi_0 \; e^{i\theta_0} \\ \phi_1 \; e^{i\theta_1} \end{pmatrix}. \tag{3}$$

Yet, for a qubit to contain only one classical bit of information, the qubit need only be unimodular (normalized to unity)

$$\alpha^*\alpha + \beta^*\beta = 1. \tag{4}$$

Hence it lives on the complex unit circle, depicted on the top of Figure 1. Normalization (4) constrains the value of the magnitudes, so we can write a qubit as

$$|q\rangle = \begin{pmatrix} \sqrt{1-f} \\ \sqrt{f} \; e^{i\varphi} \end{pmatrix}, \tag{5}$$

where $0 \le f \le 1$ and where an irrelevant overall phase is factored out. The length (or norm) of the qubit is thus an invariant quantity

$$\langle q|q\rangle = |\alpha|^2 + |\beta|^2 = |\sqrt{1-f}|^2 + |\sqrt{f}|^2 = 1. \tag{6}$$

You should understand why an overall phase is irrelevant to the length of the qubit. The quantum property of measurement follows from identifying the moduli squared of the amplitude as an occupation probability f and $1-$

[1] The names "up" and "down," and the respective symbols $|\uparrow\rangle$ and $|\downarrow\rangle$, are reserved for spin-$\frac{1}{2}$ particles.We will see in another lecture how a 2-qubit encoding conforms with the Pauli exclusion principle for particles with half-integer spin.

f for the qubit to occupy its logical states $|1\rangle$ and $|0\rangle$, respectively, as follows:

$$f = |\beta|^2 \tag{7}$$
$$1 - f = |\alpha|^2. \tag{8}$$

There are only two relevant free parameters to specify the state of a qubit, but upon measurement, the qubit originally in the superposition state (5) is found to occupy only one of its logical states

$$|q\rangle \xrightarrow{\text{measure}} \begin{cases} |1\rangle, \text{ with probability } f, \\ |0\rangle, \text{ with probability } 1-f. \end{cases} \tag{9}$$

Thus, upon a single measurement, $|q\rangle$ is found to be in either the state $|0\rangle$ or $|1\rangle$, an outcome that is said to be specified by a single classical bit $\in \{0,1\}$. Thus in actual experiments, the occupation probability f equals the frequency of occurrence of the result 1 obtained from many repeated measurements.

II. TIME-DEPENDENT QUBITS STATES

The state $|q(t)\rangle$ of a time-dependent qubit, as a two-energy level quantum mechanical entity, is governed by the Schroedinger wave equation

$$i\hbar \frac{\partial}{\partial t}|q(t)\rangle = \frac{\hbar\omega}{2}\sigma_z|q(t)\rangle. \tag{10}$$

The energy eigenvalues are $\pm\hbar\omega/2$ and energy eigenstates are

$$|0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{11}$$

where $|0\rangle$ is the ground state and $|1\rangle$ is the excited state of the qubit. In terms of the angular frequency ω (e.g. Rabi frequency), the time-dependent qubit state is

$$|q(t)\rangle = \mathcal{A}_0 e^{-i\frac{\omega}{2}t}|0\rangle + \mathcal{A}_1 e^{i\frac{\omega}{2}t}|1\rangle, \tag{12}$$

where the complex probability amplitudes satisfy $|\mathcal{A}_0|^2 + |\mathcal{A}_1|^2 = 1$ since the qubit resides on the complex circle in Hilbert space (or the Bloch sphere in spin space).

Now, we can explicitly write out qubit basis states of the Bloch sphere with $\hat{u} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ as

$$|+\rangle_u = \begin{pmatrix} \cos\frac{\theta}{2}e^{-i\frac{\varphi}{2}} \\ \sin\frac{\theta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = \cos\frac{\theta}{2}e^{-i\frac{\varphi}{2}}|0\rangle + \sin\frac{\theta}{2}e^{i\frac{\varphi}{2}}|1\rangle, \tag{13a}$$

$$|-\rangle_u = \begin{pmatrix} -\sin\frac{\theta}{2}e^{-i\frac{\varphi}{2}} \\ \cos\frac{\theta}{2}e^{i\frac{\varphi}{2}} \end{pmatrix} = -\sin\frac{\theta}{2}e^{-i\frac{\varphi}{2}}|0\rangle + \cos\frac{\theta}{2}e^{i\frac{\varphi}{2}}|1\rangle. \tag{13b}$$

Writing our 2-spinor basis states in terms of qubit states, we have

$$\xi(\uparrow) \equiv e^{i\frac{\varphi}{2}}|+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2} \end{pmatrix} = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\varphi}|1\rangle, \tag{14a}$$

$$\xi(\downarrow) \equiv e^{-i\frac{\varphi}{2}}|-\rangle = \begin{pmatrix} -e^{-i\varphi}\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix} = -\sin\frac{\theta}{2}e^{-i\varphi}|0\rangle + \cos\frac{\theta}{2}|1\rangle. \tag{14b}$$

III. QUBIT REPRESENTATIONS

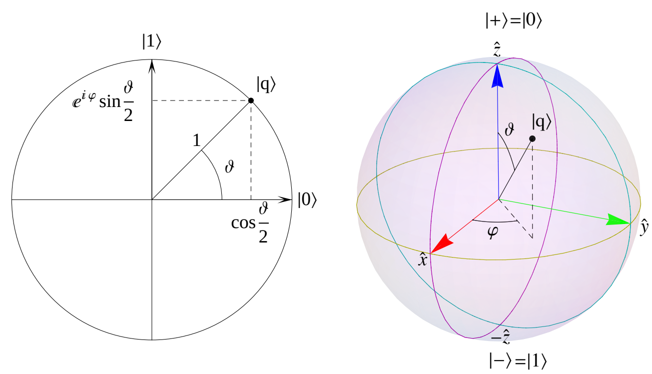

FIG. 1 A qubit in Hilbert space in its SU(2) representation (top), and the same qubit on the Bloch sphere in its O(3) representation (bottom). SU(2) and O(3) are homomorphic.

A. Hilbert space representation

The space of all possible orientations of $|q\rangle$ on the complex unit circle is called the Hilbert space. In the logical basis, the two degrees of freedom of the qubit is often expressed as two angles θ and φ, where $f = \sin^2\left(\frac{\theta}{2}\right)$. So without any loss of generality the Hilbert space representation of a qubit (1) can be written as

$$|q\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|1\rangle. \tag{15}$$

These angles have a well known geometrical interpretation as Euler angles.

B. SU(2) and O(3) representations

To understand the geometrical interpretation of a qubit, consider a three-dimensional space with "unit vectors" σ_x, σ_y, and σ_z chosen as an orthonormal basis. In quantum information theory, one represents each basis element by a 2×2 matrix, a traceless hermitian generators of two-dimensional special unitary group, SU(2). To do so, one defines the symmetric product (dot product) as

$$\sigma_i \cdot \sigma_j \equiv \frac{1}{2}\left(\sigma_i \cdot \sigma_j + \sigma_j \cdot \sigma_i\right). \tag{16a}$$

Furthermore, one defines the anti-symmetric product (cross product) as

$$\sigma_i \times \sigma_j \equiv -\frac{i}{2}\left(\sigma_i \cdot \sigma_j - \sigma_j \cdot \sigma_i\right). \tag{16b}$$

Note that the centered dot symbol on the R.H.S. of (16) denotes matrix multiplication. Thus, a basis that is orthonormal satisfies the following conditions

$$\sigma_i \cdot \sigma_j = \begin{cases} 1, \text{ for } i = j \text{ (normal)}, \\ 0, \text{ otherwise (orthogonal)}, \end{cases} \tag{17a}$$

and

$$\sigma_i \times \sigma_j = \begin{cases} 0, \text{ for } i = j, \\ \sigma_k, \text{ for cyclic indices.} \end{cases} \tag{17b}$$

A fundamental matrix representation that satisfies (17) is the well-known Pauli basis

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{18}$$

Exercise:

If it is not obvious already, verify that the Pauli matrices (18) satisfy the orthonormality conditions (17) which is just the structure equation for the SU(2) group

$$[S_i, S_j] = i\,\epsilon_{ijk}\,S_k,$$

where $S_i \equiv \frac{\sigma_i}{2}$ and the structure constant ϵ_{ijk} is the anti-symmetric Levi-Civita symbol.

Now we can express the qubit (15) in vector form (i.e. with three real components) as follows:

$$\vec{q} = (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta). \tag{19}$$

(19) is a representation of a qubit on the Bloch sphere where θ is the elevation angle and φ is the azimuthal angle. In this representation, depicted on the bottom of Fig. 1, the qubit is considered as a vector element of the three-dimensional orthogonal group, O(3). Defining the Pauli spin vector (which has matrix components)

$$\vec{\sigma} \equiv (\sigma_1, \sigma_2, \sigma_3), \tag{20}$$

a qubit can also be expressed in matrix form

$$\begin{aligned} M_q &\equiv \vec{q} \cdot \vec{\sigma} && (21a) \\ &= \sin\theta\cos\varphi\,\sigma_1 + \sin\theta\sin\varphi\,\sigma_2 + \cos\theta\,\sigma_3 && (21b) \\ &\overset{(18)}{=} \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}. && (21c) \end{aligned}$$

In this representation, the qubit is expressed as a matrix element of the SU(2) group. In quantum information, usually 2×2 unitary matrices are considered single-qubit quantum gates, but such matrices can themselves represent qubits too. Table I gives a summary of the three qubit representations

Representations	Qubit
Hilbert space	$\lvert q\rangle = \cos\left(\frac{\theta}{2}\right)\lvert 0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}\lvert 1\rangle$
O(3) group	$\vec{q} = (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta)$
SU(2) group	$M_q = \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}$

TABLE I Qubit representations.

IV. ROTATION BY SIMILARITY TRANSFORMATION

Now that we see a qubit as simply a unit vector on the complex circle (Hilbert space representation) or a unit vector on the Bloch sphere (O(3) representation), we can consider rotations of the qubit's state that keep its length (or norm) invariant. Remarkably, such a rotation of a qubit is conveniently accomplished by employing its SU(2) representation as a 2×2 unitary matrix. Then, the qubit rotation is induced by a similarity transformation, which is to say a double-sided transformation acting from the left and the right side. The unitary matrix (acting from the left) along with its matrix inverse (acting from the right) that is customarily employed for such rotations, about the ith principle axis say, is

$$U_i(\theta) \equiv e^{-i\frac{\theta}{2}\sigma_i} = \sigma_0 \cos\left(\frac{\theta}{2}\right) - i\sigma_i \sin\left(\frac{\theta}{2}\right), \tag{22}$$

where the identity matrix is $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. Explicitly, the unitary matrices for the principles directions are

$$\begin{aligned} U_1(\theta) &= \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix} && (23a) \\ U_2(\theta) &= \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix} && (23b) \\ U_3(\theta) &= \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}. && (23c) \end{aligned}$$

A general rotation of a qubit about axis $\hat{n} = (n_x, n_y, n_z)$ is built using the following unitary matrix (along with its inverse)

$$U_{\hat{n}}(\theta) = e^{-i\frac{\theta}{2}\hat{n}\cdot\vec{\sigma}} = \sigma_0 \cos\left(\frac{\theta}{2}\right) - i(\hat{n}\cdot\vec{\sigma})\sin\left(\frac{\theta}{2}\right), \tag{24}$$

where the identity on the R.H.S. follows since $(\hat{n}\cdot\vec{\sigma})^2 = \sigma_0 = \mathbf{1}$.

Now a qubit rotation by angle θ about the arbitrary axis $\hat{n}$ is expressed as the similarity transformation mentioned above

$$M_{q'} = U_{\hat{n}}(\theta) \cdot M_q \cdot U_{\hat{n}}^\dagger(\theta). \tag{25}$$

Here again the centered dot symbol represents matrix multiplication. The † symbol denotes the matrix adjoint, *i.e.* complex conjugate of the components of the matrix combined with matrix transposition. Since

$$U^\dagger_{\hat{n}}(\theta) = U^{-1}_{\hat{n}}(\theta) = U_{\hat{n}}(-\theta), \tag{26}$$

we simply compute the rotated qubit (25) as follows

$$M_{q'} \;=\; U_{\hat{n}}(\theta)\cdot M_q \cdot U_{\hat{n}}(-\theta). \tag{27}$$

Of course using $M_q = \vec{q}\cdot\vec{\sigma}$ we can write this similarity transformation directly in terms of the 3-vector $\vec{q}$ and the resulting 3-vector $\vec{q'}$

$$\vec{q'}\cdot\vec{\sigma} \;=\; U_{\hat{n}}(\theta)\cdot(\vec{q}\cdot\vec{\sigma})\cdot U_{\hat{n}}(-\theta). \tag{28}$$

The goal is to workout the R.H.S. so that we can determine $\vec{q'}$ in terms of the original vector $\vec{q}$, the axis of rotation $\hat{n}$, and the angular rotation amount θ. We will see that (28) reduces to a particularly simple and useful rotation formula.

As a preliminary task leading toward reducing (28), we will need some helpful identities. Consider two 3-vectors $\vec{a}$ and $\vec{b}$. The first identity that we need is

$$(\vec{a}\cdot\vec{\sigma})\cdot(\vec{b}\cdot\vec{\sigma}) = \vec{a}\cdot\vec{b} + i\left(\vec{a}\times\vec{b}\right)\cdot\vec{\sigma}. \tag{29}$$

The proof is simple enough and goes as follows:

$$\begin{aligned}
(\vec{a}\cdot\vec{\sigma})(\vec{b}\cdot\vec{\sigma}) &= (a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)\,(b_1\sigma_1 + b_2\sigma_2 + b_3\sigma_3) && \text{(30a)}\\
&= \vec{a}\cdot\vec{b} + a_1b_2\sigma_1\sigma_2 + b_1a_2\sigma_2\sigma_1 + \text{O.T.} && \text{(30b)}\\
&= \vec{a}\cdot\vec{b} + i(a_1b_2 - b_1a_2)\sigma_3 + \text{O.T.} && \text{(30c)}\\
&= \vec{a}\cdot\vec{b} + i\left(\vec{a}\times\vec{b}\right)\cdot\vec{\sigma}, && \text{(30d)}
\end{aligned}$$

where O.T. stands for the "other terms." In turn, it follows that

$$\begin{aligned}
(\vec{a}\cdot\vec{\sigma})\cdot(\vec{b}\cdot\vec{\sigma}) &= \vec{a}\cdot\vec{b} + i\left(\vec{a}\times\vec{b}\right)\cdot\vec{\sigma} && \text{(31a)}\\
(\vec{b}\cdot\vec{\sigma})\cdot(\vec{a}\cdot\vec{\sigma}) &= \vec{a}\cdot\vec{b} - i\left(\vec{a}\times\vec{b}\right)\cdot\vec{\sigma}. && \text{(31b)}
\end{aligned}$$

Then, taking the sum and difference yields the following two identities

$$\begin{aligned}
(\vec{a}\cdot\vec{\sigma})\cdot(\vec{b}\cdot\vec{\sigma}) + (\vec{b}\cdot\vec{\sigma})\cdot(\vec{a}\cdot\vec{\sigma}) &= 2\,\vec{a}\cdot\vec{b} && \text{(32a)}\\
(\vec{a}\cdot\vec{\sigma})\cdot(\vec{b}\cdot\vec{\sigma}) - (\vec{b}\cdot\vec{\sigma})\cdot(\vec{a}\cdot\vec{\sigma}) &= 2i\left(\vec{a}\times\vec{b}\right)\cdot\vec{\sigma}. && \text{(32b)}
\end{aligned}$$

Finally, we have the useful identity

$$(\hat{a}\cdot\vec{\sigma})\cdot(\vec{b}\cdot\vec{\sigma})\cdot(\hat{a}\cdot\vec{\sigma}) \overset{(32a)}{=} -(\vec{b}\cdot\vec{\sigma}) + 2\,(\hat{a}\cdot\vec{b})(\hat{a}\cdot\vec{\sigma}), \tag{33}$$

which follows since $(\hat{a}\cdot\vec{\sigma})^2 = 1$.

We are now in a position to accomplish the reduction of (28) which goes as follows

$$
\begin{aligned}
\vec{q'}\cdot\vec{\sigma} &= U_{\hat{n}}(\theta)\cdot(\vec{q}\cdot\vec{\sigma})\cdot U_{\hat{n}}(-\theta) && \text{(34a)}\\
&\overset{(22)}{=} \left[\sigma_0\cos\left(\frac{\theta}{2}\right) - i\sigma_i\sin\left(\frac{\theta}{2}\right)\right]\cdot(\vec{q}\cdot\vec{\sigma})\cdot\left[\sigma_0\cos\left(\frac{\theta}{2}\right) - i\sigma_i\sin\left(\frac{\theta}{2}\right)\right] && \text{(34b)}\\
&= \cos^2\left(\frac{\theta}{2}\right)(\vec{q}\cdot\vec{\sigma}) + \sin^2\left(\frac{\theta}{2}\right)(\hat{n}\cdot\vec{\sigma})\cdot(\vec{q}\cdot\vec{\sigma})\cdot(\hat{n}\cdot\vec{\sigma}) + i\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)\Big[-(\hat{n}\cdot\vec{\sigma})\cdot(\vec{q}\cdot\vec{\sigma}) + (\vec{q}\cdot\vec{\sigma})\cdot(\hat{n}\cdot\vec{\sigma})\Big] \\
&\overset{(32b)}{=} \cos^2\left(\frac{\theta}{2}\right)(\vec{q}\cdot\vec{\sigma}) + \sin^2\left(\frac{\theta}{2}\right)(\hat{n}\cdot\vec{\sigma})\cdot(\vec{q}\cdot\vec{\sigma})\cdot(\hat{n}\cdot\vec{\sigma}) + \sin\theta\,(\hat{n}\times\vec{r})\cdot\vec{\sigma} && \text{(34c)}\\
&\overset{(33)}{=} \cos^2\left(\frac{\theta}{2}\right)(\vec{q}\cdot\vec{\sigma}) + \sin^2\left(\frac{\theta}{2}\right)\Big[-(\vec{q}\cdot\vec{\sigma}) + 2\,(\hat{n}\cdot\vec{q})(\hat{n}\cdot\vec{\sigma})\Big] + \sin\theta\,(\hat{n}\times\vec{q})\cdot\vec{\sigma} && \text{(34d)}\\
&= \cos\theta\,(\vec{q}\cdot\vec{\sigma}) + 2\sin^2\left(\frac{\theta}{2}\right)(\hat{n}\cdot\vec{q})(\hat{n}\cdot\vec{\sigma}) + \sin\theta\,(\hat{n}\times\vec{q})\cdot\vec{\sigma} && \text{(34e)}\\
&= \cos\theta\,(\vec{q}\cdot\vec{\sigma}) + (1-\cos\theta)\,(\hat{n}\cdot\vec{q})(\hat{n}\cdot\vec{\sigma}) + \sin\theta\,(\hat{n}\times\vec{q})\cdot\vec{\sigma} && \text{(34f)}\\
&= [\,\cos\theta\,\vec{q} + (1-\cos\theta)\,(\hat{n}\cdot\vec{q})\,\hat{n} + \sin\theta\,\hat{n}\times\vec{q}\,]\cdot\vec{\sigma}. && \text{(34g)}
\end{aligned}
$$

Since we are free to choose our fundamental representation $\vec{\sigma}$, this identity then implies the following general rotation formula

$$\vec{q'} = \cos\theta\,\vec{q} + (1-\cos\theta)\,\hat{n}(\hat{n}\cdot\vec{q}) + \sin\theta\,\hat{n}\times\vec{q}. \tag{35}$$

This is known as Rodrigues' rotation formula.

Exercise:

Consider the tetrahedron in $\mathbb{R}^3$ centered on the origin O with vertices $P_0 = (1,1,1)$, $P_1 = (1,-1,-1)$, $P_2 = (-1,1,-1)$, and $P_3 = (-1,-1,1)$. Let T from $\mathbb{R}^3$ to $\mathbb{R}^3$ be a rotation about the axis through points O and P_2 that transforms P_1 into P_3. Find the images of the transformation of the four corners of the tetrahedron under this transformation. Hint: Use (40) with $\theta = \frac{2\pi}{3}$ where $\hat{n}$ is directed along $P_2 - O$.

As a check of the rotation formula (35), consider the two cases when $\hat{n}\perp\vec{q}$ and $\hat{n}\parallel\vec{q}$:

$$\vec{q'} = \begin{cases} \cos\theta\,\vec{q} + \sin\theta\,\hat{n}\times\vec{q} & \text{for } \hat{n}\perp\vec{q},\\ \cos\theta\,\vec{q} + (1-\cos\theta)\,\hat{n}(\hat{n}\cdot\vec{q}) = \vec{q} & \text{for } \hat{n}\parallel\vec{q}, \end{cases} \tag{36}$$

which is correct by inspection.

V. ROTATION TRANSFORMATION IN EXPONENTIAL FORM

Writing this in component form ${q'}_i = R_{ij}(\theta)\,q_j$ we have

$$q'_i = [\cos\theta\;\delta_{ij} + (1-\cos\theta)\,n_i n_j + \sin\theta\;n_k\epsilon_{ikj}]\,q_j, \tag{37}$$

whence the transformation matrix for rotations about $\hat{n}$ is immediately identified

$$
\begin{aligned}
R_{\hat{n}}(\theta) &= \begin{pmatrix} \cos\theta + (1-\cos\theta)\, n_1^2 & (1-\cos\theta)\, n_1 n_2 - \sin\theta\, n_3 & (1-\cos\theta)\, n_1 n_3 + \sin\theta\, n_2 \\ (1-\cos\theta)\, n_1 n_2 + \sin\theta\, n_3 & \cos\theta + (1-\cos\theta)\, n_2^2 & (1-\cos\theta)\, n_2 n_3 - \sin\theta\, n_1 \\ (1-\cos\theta)\, n_1 n_3 - \sin\theta\, n_2 & (1-\cos\theta)\, n_2 n_3 + \sin\theta\, n_1 & \cos\theta + (1-\cos\theta)\, n_3^2 \end{pmatrix} && \text{(38a)} \\
&= \cos\theta\, \mathbf{1}_3 + (1-\cos\theta) \begin{pmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_1 n_2 & n_2^2 & n_2 n_3 \\ n_1 n_3 & n_2 n_3 & n_3^2 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} && \text{(38b)} \\
&= \cos\theta\, \mathbf{1}_3 + (1-\cos\theta) \begin{pmatrix} 1-n_2^2-n_3^2 & n_1 n_2 & n_1 n_3 \\ n_1 n_2 & 1-n_1^2-n_3^2 & n_2 n_3 \\ n_1 n_3 & n_2 n_3 & 1-n_1^2-n_2^2 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} && \text{(38c)} \\
&= \mathbf{1}_3 + (1-\cos\theta) \begin{pmatrix} -n_2^2-n_3^2 & n_1 n_2 & n_1 n_3 \\ n_1 n_2 & -n_1^2-n_3^2 & n_2 n_3 \\ n_1 n_3 & n_2 n_3 & -n_1^2-n_2^2 \end{pmatrix} + \sin\theta \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} && \text{(38d)} \\
&= \mathbf{1}_3 + (1-\cos\theta)\, \lambda^2 + \sin\theta\, \lambda, && \text{(38e)}
\end{aligned}
$$

where the generator $\lambda_{ij} \equiv \epsilon_{ikj} n_k$ of a rotation about $\hat{n}$ is the anti-symmetric matrix

$$
\lambda \equiv \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}, \tag{39}
$$

which is skew tri-idempotent (*i.e.* $\lambda^3 = -\lambda$). Thus, we can write the rotation matrix in exponential form

$$
R_{\hat{n}}(\theta) = e^{\theta\lambda}. \tag{40}
$$

The determinant $\det[R_{\hat{n}}(\theta)] = 1$, so the traceless hermitian matrices spaning (39)

$$
\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},
$$

are generators of the SO(3) group. This leads one to define three traceless hermitian matrices

$$
J_1 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad J_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \qquad J_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \tag{41}
$$

which are tri-idempotent ($J_i^3 = J_i$). Thus, the rotation matrix (40) takes on a manifestly unitary form

$$
R_{\hat{n}}(\theta) = e^{-i\theta(n_1 J_3 + n_2 J_2 + n_3 J_1)}. \tag{42}
$$

The labeling of the components of the rotation axis is arbitrary. By relabeling to match the generators, $n_1 \to A_3$, $n_2 \to A_2$, and $n_3 \to A_1$, we can write (42) as a rotation about $\hat{A}$

$$
R_{\hat{A}}(\theta) = e^{-i\theta(\hat{A}\cdot\vec{J})}. \tag{43}
$$

With this particular choice of generators, (41) is a 3×3 adjoint representation of SU(2)

$$
[J_l, J_m] = i\,\epsilon_{lmn} J_n. \tag{44}
$$

(41) is also an irreducible spin-1 representation of SU(2).

VI. COMPOSITION OF QUBIT ROTATIONS

A rotation through angle β_1 about $\hat{n}_1$, followed by a rotation through angle β_2 about $\hat{n}_2$ is induced by a similarity transformation using a unitary matrix that is the composition

$$\begin{aligned}
U_{\hat{n}_2}(\beta_2)U_{\hat{n}_1}(\beta_1) &= e^{-i\frac{\beta_2}{2}\hat{n}_2\cdot\vec{\sigma}}e^{-i\frac{\beta_1}{2}\hat{n}_1\cdot\vec{\sigma}} && \text{(45a)}\\
&= \left[\cos\frac{\beta_2}{2} - i(\hat{n}_2\cdot\vec{\sigma})\sin\frac{\beta_2}{2}\right]\left[\cos\frac{\beta_1}{2} - i(\hat{n}_1\cdot\vec{\sigma})\sin\frac{\beta_1}{2}\right] && \text{(45b)}\\
&= \cos\frac{\beta_1}{2}\cos\frac{\beta_2}{2} - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}(\hat{n}_1\cdot\vec{\sigma})(\hat{n}_2\cdot\vec{\sigma})\\
&- i\left[\cos\frac{\beta_1}{2}\sin\frac{\beta_2}{2}(\hat{n}_2\cdot\vec{\sigma}) + \sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2}(\hat{n}_1\cdot\vec{\sigma})\right]. && \text{(45c)}
\end{aligned}$$

We need to expand the double dot product term in (45c). To do this, we use the identity (29) that we already derived above. Thus,

$$\begin{aligned}
U_{\hat{n}_2}(\beta_2)U_{\hat{n}_1}(\beta_1) &= \cos\frac{\beta_1}{2}\cos\frac{\beta_2}{2} - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{n}_1\cdot\hat{n}_2 && \text{(46)}\\
&- i\left[\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2}\hat{n}_1 + \cos\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{n}_2 - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{n}_1\times\hat{n}_2\right]\cdot\vec{\sigma}.
\end{aligned}$$

The overall unitary matrix used to induce a rotation through β_{12} about $\hat{n}_{12}$ is

$$U_{\hat{n}_{12}}(\beta_{12}) = e^{-i\frac{\beta_{12}}{2}\hat{n}_{12}\cdot\vec{\sigma}} = \cos\frac{\beta_{12}}{2} - i\sin\frac{\beta_{12}}{2}\hat{n}_{12}\cdot\vec{\sigma}. \tag{47}$$

Finally, equating our two expressions for the unitary matrices, (46)=(47), which is

$$U_{\hat{n}_{12}}(\beta_{12}) = U_{\hat{n}_2}(\beta_2)U_{\hat{n}_1}(\beta_1), \tag{48}$$

the real and imaginary parts lead to the following two identities

$$\begin{aligned}
\cos\frac{\beta_{12}}{2} &= \cos\frac{\beta_1}{2}\cos\frac{\beta_2}{2} - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{n}_1\cdot\hat{n}_2 && \text{(49a)}\\
\sin\frac{\beta_{12}}{2}\hat{n}_{12} &= \sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2}\hat{n}_1 + \cos\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{n}_2 - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{n}_1\times\hat{n}_2. && \text{(49b)}
\end{aligned}$$

A. Special case of equal angles

For equal angles $\beta_1 = \beta_2 = \frac{\Delta t}{2}$, and making the following identifications for the rotation axes

$$\hat{n}_1 = \hat{\psi} \quad \text{and} \quad \hat{n}_2 = \hat{z}, \tag{50}$$

(49) reduces to an identity that we will use to prove the efficiency of Grover's quantum search algorithm

$$\begin{aligned}
\cos\frac{\beta_{12}}{2} &= \cos^2\frac{\Delta t}{2} - \sin^2\frac{\Delta t}{2}\hat{\psi}\cdot\hat{z} && \text{(51a)}\\
\sin\frac{\beta_{12}}{2}\hat{n}_{12} &= \sin\frac{\Delta t}{2}\cos\frac{\Delta t}{2}\left(\hat{\psi}+\hat{z}\right) - \sin^2\frac{\Delta t}{2}\hat{\psi}\times\hat{z}. && \text{(51b)}
\end{aligned}$$

VII. EXAMPLE COMPOSITE ROTATION

Consider a local evolution operator as a composition of "qubit rotations" $U_{\hat{\boldsymbol{n}}_2} = e^{-i\frac{\beta_2}{2}\hat{\boldsymbol{n}}_2\cdot\boldsymbol{\sigma}}$ and $U_{\hat{\boldsymbol{n}}_1} = e^{-i\frac{\beta_1}{2}\hat{\boldsymbol{n}}_1\cdot\boldsymbol{\sigma}}$:

$$\begin{aligned}
U_{\hat{\boldsymbol{n}}_2}(\beta_2)U_{\hat{\boldsymbol{n}}_1}(\beta_1) &= e^{-i\frac{\beta_2}{2}\hat{\boldsymbol{n}}_2\cdot\boldsymbol{\sigma}}e^{-i\frac{\beta_1}{2}\hat{\boldsymbol{n}}_1\cdot\boldsymbol{\sigma}} && \text{(52a)}\\
&= \cos\frac{\beta_1}{2}\cos\frac{\beta_2}{2} - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{\boldsymbol{n}}_1\cdot\hat{\boldsymbol{n}}_2\\
&- i\Big[\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2}\hat{\boldsymbol{n}}_1 + \cos\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{\boldsymbol{n}}_2\\
&\quad - \sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\hat{\boldsymbol{n}}_1\times\hat{\boldsymbol{n}}_2\Big]\cdot\boldsymbol{\sigma}, && \text{(52b)}
\end{aligned}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a vector of Pauli matrices, $\hat{\boldsymbol{n}}_1$ and $\hat{\boldsymbol{n}}_2$ are unit vectors specifying the respective principal axes of rotation, and β_1 and β_2 are real-valued rotation angles. Let us take $U_{\text{S}}^z = e^{-i\frac{\beta_2}{2}\hat{\boldsymbol{n}}_2\cdot\boldsymbol{\sigma}}$ as our stream operator and $U_{\text{C}} = e^{-i\frac{\beta_1}{2}\hat{\boldsymbol{n}}_1\cdot\boldsymbol{\sigma}}$ as our collision operator. Let us choose a reference frame where the particle motion occurs along the $\hat{\boldsymbol{z}}$

$$U_{\text{S}}^z = e^{-i\frac{\beta_2}{2}\sigma_z}. \tag{53a}$$

In this frame a general collision operator is

$$U_{\rm C} = e^{-i\frac{\beta_1}{2}(\alpha\sigma_x+\beta\sigma_y+\gamma\sigma_z)}, \tag{53b}$$

where α, β, and γ are real valued components subject to the constraint $\alpha^2+\beta^2+\gamma^2=1$. Furthermore, let us suppose that the unitary operators (53) are applied locally and homogeneously at all the points in the system. So, here we consider a construction whereby the two principal unit vectors specifying the axes of rotation are

$$\hat{\boldsymbol{n}}_1 \;=\; (\alpha,\beta,\gamma) \qquad\qquad \hat{\boldsymbol{n}}_2 = (0,0,1). \tag{54}$$

With this choice, $\hat{\boldsymbol{n}}_1\times\hat{\boldsymbol{n}}_2 = (\beta,-\alpha,0)$ and $\hat{\boldsymbol{n}}_1\cdot\hat{\boldsymbol{n}}_2=\gamma$, so (52) is a quite general representation of a quantum lattice gas evolution operator

$$\begin{aligned}
U_{\rm S}^z\, U_{\rm C} \;&\overset{(54)}{=}\; \cos\frac{\beta_1}{2}\cos\frac{\beta_2}{2} - \gamma\sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2} && \text{(55a)}\\
&- \; i\left(\alpha\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2} - \beta\sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\right)\sigma_x\\
&- \; i\left(\beta\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2} + \alpha\sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\right)\sigma_y\\
&- \; i\left(\gamma\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2} + \cos\frac{\beta_1}{2}\sin\frac{\beta_2}{2}\right)\sigma_z\\
&\mapsto \; 1 + \frac{ic\,p_z\tau}{\hbar}\sigma_z - \frac{im_\circ c^2\tau}{\hbar}\sigma_x, && \text{(55b)}
\end{aligned}$$

where the last line is chosen as a construction. The reason for choosing this construction is that the quantum algorithm $\psi' = U_{\rm S}^z\, U_{\rm C}\psi$ is

$$\psi'(z) = \left(1 + \frac{ic\,p_z\tau}{\hbar}\sigma_z - \frac{im_\circ c^2\tau}{\hbar}\sigma_x\right)\psi(z), \tag{56}$$

which is a time-difference representation of the equation of motion of a single free Dirac particle with a 2-spinor quantum state $\psi(z) = (\psi_{\rm L}(z),\psi_{\rm R}(z))^{\rm T}$ defined over the set of points $\{z\}$ in a 1+1 dimensional spacetime. That is, for small τ and for momentum operator $p_z=-i\hbar\partial_z$, (56) represents the Dirac equation for a relativistic quantum particle of mass $m_\circ$

$$i\hbar\partial_t\psi = -c\,p_z\sigma_z\psi + m_\circ c^2\sigma_x\psi. \tag{57}$$

To establish a correspondence between (55a) and (55b), we simply choose the real-valued components of $\hat{\boldsymbol{n}}_1$ to satisfy the following three conditions:

$$\begin{aligned}
\alpha\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2} \;&-\; \beta\sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2} = \frac{m_\circ c^2\tau}{\hbar} && \text{(58a)}\\
\beta\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2} \;&+\; \alpha\sin\frac{\beta_1}{2}\sin\frac{\beta_2}{2} = 0 && \text{(58b)}\\
\gamma\sin\frac{\beta_1}{2}\cos\frac{\beta_2}{2} \;&+\; \cos\frac{\beta_1}{2}\sin\frac{\beta_2}{2} = -\frac{c\,p_z\tau}{\hbar}. && \text{(58c)}
\end{aligned}$$

Additionally, we should respect the reality condition that $\hat{\boldsymbol{n}}_1$ have unit norm

$$\alpha^2+\beta^2+\gamma^2=1 \tag{58d}$$

that we established above with the collision operator (53b). For the sake of simplicity, let us start with a specialized construction whereby $\hat{\boldsymbol{n}}_1$ is perpendicular to $\hat{\boldsymbol{n}}_2$. The solution of (58) in this special case is

$$\alpha = \cos\frac{\beta_2}{2} \qquad \beta = -\sin\frac{\beta_2}{2} \qquad \gamma = 0. \tag{59}$$

Inserting (59) into (58a) gives

$$\sin\frac{\beta_1}{2} = \frac{m_\circ c^2\tau}{\hbar}, \tag{60}$$

and in turn (58c) is

$$\sqrt{1-\left(\frac{m_\circ c^2\tau}{\hbar}\right)^2}\,\sin\frac{\beta_2}{2} = -\frac{c\,p_z\tau}{\hbar}. \tag{61}$$

In turn, we have

$$\begin{aligned}
\cos\frac{\beta_1}{2}\cos\frac{\beta_2}{2} \;&=\; \sqrt{1-\left(\frac{m_\circ c^2\tau}{\hbar}\right)^2}\sqrt{1-\frac{\left(\frac{c\,p_z\tau}{\hbar}\right)^2}{1-\left(\frac{m_\circ c^2\tau}{\hbar}\right)^2}} && \text{(62a)}\\
&=\; \sqrt{1-\left(\frac{m_\circ c^2\tau}{\hbar}\right)^2-\left(\frac{c\,p_z\tau}{\hbar}\right)^2} && \text{(62b)}\\
&=\; \sqrt{1-\left(\frac{E\tau}{\hbar}\right)^2}, && \text{(62c)}
\end{aligned}$$

with $E^2=(m_\circ c^2)^2+(c\,p_z)^2$. Therefore, the quantum lattice gas evolution operator (55a) is

$$\begin{aligned}
U_{\rm S}^z\, U_{\rm C} \;&=\; \sqrt{1-\left(\frac{E\tau}{\hbar}\right)^2} + \frac{ic\,p_z\tau}{\hbar}\sigma_z - \frac{im_\circ c^2\tau}{\hbar}\sigma_x && \text{(63a)}\\
&=\; \sqrt{1-\left(\frac{E\tau}{\hbar}\right)^2} + \frac{iE\tau}{\hbar}\left(\frac{c\,p_z}{E}\sigma_z - \frac{m_\circ c^2}{E}\sigma_x\right). && \text{(63b)}
\end{aligned}$$

This result leads us to define the rotation axis

$$\hat{\boldsymbol{n}}_{12} \equiv -\frac{m_\circ c^2}{E}\,\hat{\boldsymbol{x}} + \frac{c\,p_z}{E}\,\hat{\boldsymbol{z}}. \tag{64}$$

Since $(\hat{\boldsymbol{n}}_{12}\cdot\boldsymbol{\sigma})^2 = \mathbf{1}$ (an involution), we can employ Euler's identity and the trigonometric identity $\sin(\cos^{-1}\sqrt{1-x^2}) = x$, so we are free to write (63b) in a manifestly unitary form $e^{-i\frac{\beta_{12}}{2}\hat{\boldsymbol{n}}_{12}\cdot\boldsymbol{\sigma}}$ as follows:

$$\begin{aligned}
U_{\rm S}^z U_{\rm C} &= \exp\left[i\cos^{-1}\left(\sqrt{1-\left(\frac{E\tau}{\hbar}\right)^2}\right)\hat{\boldsymbol{n}}_{12}\cdot\boldsymbol{\sigma}\right] && \text{(65a)}\\
&\overset{(64)}{=} \exp\left[i\,\frac{\cos^{-1}\sqrt{1-\left(\frac{E\tau}{\hbar}\right)^2}}{E}\left(\sigma_z c\,p_z - \sigma_x\, m_\circ c^2\right)\right]. && \text{(65b)}
\end{aligned}$$

The hermitian generator governing the dynamical behavior of the 2-spinor field ψ is the Dirac Hamiltonian

$$h_{\rm D} = -\sigma_z c\, p_z + \sigma_x\, m_\circ c^2 \tag{65c}$$

This is a remarkable finding because nowhere in the derivation of (65b) did we invoke the continuum limit where $\tau \to 0$. That is, τ may be taken to be a small but finite quantity, not necessarily infinitesimal. Thus, because of the form of (65c), Lorentz invariance would apply to the quantum dynamics even though the spacetime is discrete, albeit there are unexpected deviations from relativistic quantum mechanics (Yepez, 2010). The rotation angle in (65b) is a real scalar quantity, so we may denote this as ℓ and write

$$U_{\rm S}^z U_{\rm C} \;\cong\; e^{-i\,\ell\, h_{\rm D}/(\hbar c)}, \tag{65d}$$

where in the last line we made the identification

$$\cos\left(\frac{E\ell}{\hbar c}\right) = \sqrt{1-\left(\frac{E\tau}{\hbar}\right)^2}, \tag{66}$$

or expressing τ in terms of the grid size ℓ

$$\tau = \frac{\hbar}{E}\sin\left(\frac{E\ell}{\hbar c}\right). \tag{67}$$

References

Yepez, J., 2010, arXiv:1106.0739 [gr-qc] .