QUANTUM MECHANICS FOUNDATIONS OF QUANTUM INFORMATION PROCESSING

DYNAMICS

THIRD POSTULATE
(Time Evolution)

The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

where $\hat{H}(t)$ is the observable associated with the total energy of the system.

Formal solution of the Schrödinger equation:

(i) Time-dependent Hamiltonian

$$|\psi(t)\rangle \;=\; \mathcal{T} e^{-\frac{i}{\hbar} \int_0^t \hat{H}(t')\, dt'} |\psi(0)\rangle = \hat{U}_t\, |\psi(0)\rangle$$

where $\mathcal{T}$ is a time ordering operator.

(ii) Time-independent Hamiltonian

$$|\psi(t)\rangle \;=\; e^{-\frac{i}{\hbar} \hat{H} t} |\psi(0)\rangle = \hat{U}_t\, |\psi(0)\rangle$$

The operator $\hat{U}_t$ is called **evolution operator** or **propagator**. It evolves or propagates state of a quantum mechanical system from the initial time $t' = 0$ to a final time $t' = t$.

Since the Hamiltonian is self-adjoined, the evolution operator is **unitary**:

$$\hat{U}_t = e^{-\frac{i}{\hbar}\hat{H}t}$$

$$\hat{U}_t^\dagger = e^{\frac{i}{\hbar}\hat{H}t} = \hat{U}_{-t} = \hat{U}_t^{-1}$$

$$\hat{U}_t\hat{U}_t^\dagger = e^{-\frac{i}{\hbar}\hat{H}t}\, e^{\frac{i}{\hbar}\hat{H}t} = \hat{U}_t^\dagger\hat{U}_t = e^{\frac{i}{\hbar}\hat{H}t}\, e^{-\frac{i}{\hbar}\hat{H}t} = \hat{I}$$

The evolution operator can also evolve the state given by a density operator. Since $|\psi(t)\rangle = \hat{U}_t|\psi(0)\rangle$ and the adjoint is $\langle\psi(t)| = \langle\psi(0)|\hat{U}_t^\dagger$, the density matrix at time t is given as

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = \hat{U}_t\,|\psi(0)\rangle\langle\psi(0)|\,\hat{U}_t^\dagger = \hat{U}_t\,\rho(0)\,\hat{U}_t^\dagger$$

Example: A two-level atom

Let us have an atoms with two energy levels separated by the energy $\hbar\omega$:

$$\begin{aligned} E_- &= -\hbar\omega/2 \\ E_+ &= +\hbar\omega/2 \end{aligned}$$

In the representation given by the corresponding eigenvectors, $|E_-\rangle$ and $|E_+\rangle$ respectively, the Hamiltonian is

$$\hat{H} = \frac{\hbar\omega}{2}\,\sigma_z$$

and the evolution operator then reads as

$$\hat{U}_t = e^{-\frac{i}{\hbar}\,\hat{H}t} = e^{-i\,\omega\,t\,\sigma_z/2} = \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix}$$

Connecting with Bloch representation

We can rewrite the evolution operator above as

$$\begin{aligned}\hat{U}_t &= \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix} = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix} \\ &= \begin{pmatrix} \cos\theta/2 & 0 \\ 0 & \cos\theta/2 \end{pmatrix} - i \begin{pmatrix} \sin\theta/2 & 0 \\ 0 & -\sin\theta/2 \end{pmatrix} \\ &= \cos\frac{\theta}{2}\,\hat{I} - i\sin\frac{\theta}{2}\,\sigma_z = \hat{R}_z(\theta)\end{aligned}$$

and examine its action on a qubit $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$, where $|0\rangle = |E_-\rangle$ and $|1\rangle = |E_+\rangle$, whose initial state is given by the density matrix in the Bloch representation

$$\rho(0) = \frac{1}{2}\left(\hat{I} + \vec{r}(0)\,.\,\vec{\sigma}\right)$$

We evaluate the action of the evolution operator as follows

$$
\begin{aligned}
\rho(t) &= \hat{U}_t\,\rho(0)\,\hat{U}_t^{\dagger} = \hat{R}_z(\theta)\,\rho(0)\,\hat{R}_z^{\dagger}(\theta) = \hat{R}_z(\theta)\left[\frac{1}{2}\left(\hat{I} + \vec{r}(0)\,.\,\vec{\sigma}\right)\right]\hat{R}_z^{\dagger}(\theta) \\
&= \frac{1}{2}\left(\hat{I} + \hat{R}_z(\theta)\vec{r}(0)\,.\,\vec{\sigma}\hat{R}_z^{\dagger}(\theta)\right) \\
&= \frac{1}{2}\left[\hat{I} + \left(\cos\frac{\theta}{2}\,\hat{I} - i\sin\frac{\theta}{2}\,\sigma_z\right)\left(r_x\sigma_x + r_y\sigma_y + r_z\sigma_z\right)\left(\cos\frac{\theta}{2}\,\hat{I} + i\sin\frac{\theta}{2}\,\sigma_z\right)\right] \\
&= \frac{1}{2}\left[\hat{I} + (r_x\cos\theta - r_y\sin\theta)\,\sigma_x + (r_x\sin\theta + r_y\cos\theta)\,\sigma_y + r_z\,\sigma_z\right]
\end{aligned}
$$

We observe that it causes the rotation of the Bloch vector around the axis z by the angle θ:

$$
\vec{r}(0) = (r_x, r_y, r_z) \quad\rightarrow\quad \vec{r}(t) = (r_x\cos\theta - r_y\sin\theta, r_x\sin\theta + r_y\cos\theta, r_z)
$$

Similarly, we can define the rotation operators about any axis in the Bloch representation

$$
\begin{aligned}
\hat{R}_x(\theta) &= e^{-i\theta\sigma_x/2} = \cos\frac{\theta}{2}\,\hat{I} - i\sin\frac{\theta}{2}\,\sigma_x = \begin{pmatrix} \cos\theta/2 & -i\sin\theta/2 \\ -i\sin\theta/2 & \cos\theta/2 \end{pmatrix} \\
\hat{R}_y(\theta) &= e^{-i\theta\sigma_y/2} = \cos\frac{\theta}{2}\,\hat{I} - i\sin\frac{\theta}{2}\,\sigma_y = \begin{pmatrix} \cos\theta/2 & -\sin\theta/2 \\ \sin\theta/2 & \cos\theta/2 \end{pmatrix} \\
\hat{R}_z(\theta) &= e^{-i\theta\sigma_z/2} = \cos\frac{\theta}{2}\,\hat{I} - i\sin\frac{\theta}{2}\,\sigma_z = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}
\end{aligned}
$$

Using the Taylor expansion of exponential function and properties of the Pauli operators, we can show that the operator for rotation by an angle θ about an axis defined by a real unit vector $\vec{n}$ is

$$\begin{aligned}
\hat{R}_{\vec{n}}(\theta) &= e^{-i\theta\,\vec{n}\,.\,\vec{\sigma}\,/2} \\
&= \cos\frac{\theta}{2}\,\hat{I} - i\sin\frac{\theta}{2}\,\vec{n}\,.\,\vec{\sigma} \\
&= \begin{pmatrix} \cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2} & -in_x\sin\frac{\theta}{2} - n_y\sin\frac{\theta}{2} \\ -in_x\sin\frac{\theta}{2} + n_y\sin\frac{\theta}{2} & \cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2} \end{pmatrix}
\end{aligned}$$

Properties of the set of all unitary operators $\hat{R}_{\vec{n}}(\theta)$:

1. product of two operators from this set is again a unitary operator

$$\begin{aligned}\hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta')\left(\hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta')\right)^{\dagger} &= \hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta')\hat{R}^{\dagger}_{\vec{n}'}(\theta')\hat{R}^{\dagger}_{\vec{n}}(\theta) = \hat{I}\\ \left(\hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta')\right)^{\dagger}\hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta') &= \hat{R}^{\dagger}_{\vec{n}'}(\theta')\hat{R}^{\dagger}_{\vec{n}}(\theta)\hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta') = \hat{I};\end{aligned}$$

   ad since it is a product of two rotations in the Bloch representation we can trust that the product itself also corresponds to a rotation and is therefore an element of the same set.

Baker-Campbell-Hausdorff formula

It is to be said that we can **not** in general rewrite the product $\hat{R}_{\vec{n}}(\theta)\hat{R}_{\vec{n}'}(\theta')$ above as a single exponential function. In the non-commutative world, the product of two exponential functions of non-commuting operators is **not** an exponential function of the sum of the two operators. Instead the product is given by the **Baker-Campbell-Hausdorff formula** which for two non-commuting operators $\hat{A}$ and $\hat{B}$ reads as

$$e^{\hat{A}}\ e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\frac{1}{12}([\hat{A},[\hat{A},\hat{B}]]+[[\hat{A},\hat{B}],\hat{B}])+\ldots}$$

2. The set contains an identity operator $\hat{R}_{\vec{n}}(\theta = 0) = \hat{I}$.

3. every element of the set $\hat{R}_{\vec{n}}(\theta)$ has an inverse $\hat{R}_{\vec{n}}^{\dagger}(\theta) = \hat{R}_{\vec{n}}^{-1}(\theta)$;

4. every element of the set has the unit determinant: $\det \hat{R}_{\vec{n}}(\theta) = 1$.

The properties above contain the group axioms. The set of unitary operators $\hat{R}_{\vec{n}}(\theta)$ hence forms a group, specifically, of 2-by-2 unitary matrices of unit determinant, called

the special unitary group $SU(2)$**.**

$SU(2)$ is a Lie group

A **Lie group** is a group which is also a smooth manifold G. The neighborhood of any point of a Lie group, considered as a manifold, looks exactly like that of any other. Thus the group dimension and much of its structure can be understood by examining the immediate vicinity of any chosen point, for instance, the identity element.

Example: a near identity element of the general linear group $GL(n, \mathbb{R})$, which consists of invertible n-by-n real matrices, can be written as $g = I + \epsilon A$ where A is an arbitrary n-by-n matrix. This matrix consists of n^2 entries and therefore the group manifold itself is n^2 dimensional. $GL(n, \mathbb{C})$ has $2n^2$ real dimensions.

The special linear group $SL(n, \mathbb{R})$ consists of elements of $GL(n, \mathbb{R})$ characterized by the unit determinant $\det g = 1$. For the element near identity $g = I + \epsilon A$ this implies that $\mathrm{tr}\, A = 0$ as $\det(I + \epsilon A) = 1 + \epsilon\ \mathrm{tr}\, A + O(\epsilon^2)$. Consequently $SL(n, \mathbb{R})$ is $n^2 - 1$ dimensional. The dimension of $SU(n)$ is also $n^2 - 1$, so $SU(2)$ is three dimensional as a manifold.

The vectors lying in the tangent space at the identity element make up the **Lie algebra** of the group. We say that the Lie group is generated by its Lie algebra.

Example: $SU(2)$
The Taylor expansion of $\hat{R}_{\vec{n}}(\theta) \in SU(2)$ to the first order in small $\theta = \epsilon$ is

$$\hat{R}_{\vec{n}}(\epsilon) = e^{-i\epsilon\, \vec{n}\, .\, \vec{\sigma}\, /2} = \hat{I} - i\epsilon \left(n_x \frac{\sigma_x}{2} + n_y \frac{\sigma_y}{2} + n_z \frac{\sigma_z}{2} \right) + O(\epsilon^2)$$

where the expression in the bracket on r.h.s. is an element of the $su(2)$ algebra and $T_a = \frac{\sigma_a}{2}$ where $a = x, y, z$ are its generators.

More generally, the Lie algebra generators can be obtained from the group elements $g \in G$ directly. In our case, we introduce $\vec{\theta} = \theta\,\vec{n} = (\theta n_x, \theta n_y, \theta n_z) = (\theta_x, \theta_y, \theta_z)$ and identify $g\left(\vec{\theta}\right) = \hat{R}_{\vec{n}}(\theta)$. The generators are then obtained by through the following expression

$$T_a = i\, g^{-1}\left(\vec{\theta}\right)\, \frac{\partial g\left(\vec{\theta}\right)}{\partial \theta_a}$$

Explicitely:

$$\begin{aligned}
T_x &= i\, e^{i\left(\theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z\right)/2}\, \frac{\partial}{\partial\theta_x} e^{-i\left(\theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z\right)/2} = \frac{\sigma_x}{2} \\
T_y &= i\, e^{i\left(\theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z\right)/2}\, \frac{\partial}{\partial\theta_y} e^{-i\left(\theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z\right)/2} = \frac{\sigma_y}{2} \\
T_z &= i\, e^{i\left(\theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z\right)/2}\, \frac{\partial}{\partial\theta_z} e^{-i\left(\theta_x\sigma_x + \theta_y\sigma_y + \theta_z\sigma_z\right)/2} = \frac{\sigma_z}{2}
\end{aligned}$$

The generators of $su(2)$ algebra are indeed similar to the operators for components of the spin angular momentum of a spin-1/2 particle, up to the scaling by $\hbar$.

They also satisfy the same commutation, known as the **Lie bracket**,

$$[T_a, T_b] \;=\; i\epsilon_{abc}\, T_c$$

where ϵ_{abc} is the Levi-Civita tensor.

The Lie bracket is antisymmetric, $[X, Y] = -[Y, X]$, linear, $[\lambda X + \mu Y, Z] = \lambda\,[X, Z] + \mu\,[Y, Z]$, and obeys the Jacobi identity $[[X, Y]\,, Z] + [[Y, Z]\,, X] + [[Z, X]\,, Y] = 0$.

The generators T_a satisfy the following anticommutation relations:

$$\{T_a, T_b\} \;=\; \delta_{ab}\, \hat{I}$$

Single-qubit operations are in $U(2)$

$U(2)$ is the group of 2-by-2 unitary matrices or operators. In contrast to the elements $SU(2)$, the determinant of the elements of the group $u \in U(2)$ is not fixed to unity. Each element $u \in U(2)$ can be expressed in terms of an element of $SU(2)$ as

$$u = e^{i\alpha} g$$

where $g \in SU(2)$. The exponential function involving $\alpha \in \mathbb{R}$ will shift a global phase of the qubit state. To see this we rewrite the exponential term as $e^{i\alpha} = \left(e^{i\alpha}\hat{I}\right)$. Considering the determinant of the product of two n-by-n matrices A and B, $\det(AB) = \det A \det B$, and the determinant $\det\left(e^{i\alpha}\hat{I}\right) = e^{i2\alpha}$ we obtain the map from the elements of $U(2)$ and $SU(2)$

$$g = \frac{u}{\sqrt[2]{\det u}}$$

In general, for $u \in U(n)$ we get $g = u/\sqrt[n]{\det u}$ with $g \in SU(n)$.

Examples:

(i) Phase flip

$$\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = e^{i\pi/2} \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = e^{i\pi/2} e^{-i\pi\sigma_z/2}$$

The nontrivial term $e^{-i\pi\sigma_z/2}$ on r.h.s. can be implemented via quantum evolution under the Hamiltonian $\hat{H} = \hbar\omega\sigma_z/2$ for time of the duration given by $t = \pi/\omega$:

$$\hat{U}_{t=\pi/\omega} = e^{-\frac{i}{\hbar}\hat{H}t} = e^{-i\,\omega\,\frac{\pi}{\omega}\,\sigma_z/2} = e^{-i\pi\sigma_z/2}$$

(ii) Bit flip

$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = e^{i\pi/2} \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = e^{i\pi/2} e^{-i\pi\sigma_x/2} = e^{i\pi/2} \begin{pmatrix} \cos\pi/2 & -i\sin\pi/2 \\ -i\sin\pi/2 & \cos\pi/2 \end{pmatrix}$$

(iii) Phase-bit fip $\hat{Y}$

$$\hat{Y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = e^{i\pi/2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = e^{i\pi/2} e^{-i\pi\sigma_y/2} = e^{i\pi/2} \begin{pmatrix} \cos\pi/2 & -\sin\pi/2 \\ \sin\pi/2 & \cos\pi/2 \end{pmatrix}$$

The operations above can be implemented via evolution under the appropriate Hamiltonian operators for proper duration of time.

(iv) $\hat{S} = \sqrt{\hat{Z}}$

$$\hat{S} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = e^{i\pi/4} \begin{pmatrix} e^{-i\pi/4} & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} = e^{i\pi/4} e^{-i\pi\sigma_z/4}$$

where $e^{i\pi/4} = \sqrt{\det \hat{S}}$.

(v) $\hat{T} = \sqrt{\hat{S}}$

$$\hat{T} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} = e^{i\pi/8} \begin{pmatrix} e^{-i\pi/8} & 0 \\ 0 & e^{i\pi/8} \end{pmatrix} = e^{i\pi/8} e^{-i\pi\sigma_z/8}$$

where $e^{i\pi/8} = \sqrt{\det \hat{T}}$.

(vi) Hadamard gate

$$\begin{aligned}
\hat{H} &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = e^{i\pi/2} \begin{pmatrix} \frac{e^{-i\pi/2}}{\sqrt{2}} & \frac{e^{-i\pi/2}}{\sqrt{2}} \\ \frac{e^{-i\pi/2}}{\sqrt{2}} & \frac{e^{i\pi/2}}{\sqrt{2}} \end{pmatrix} \\
&= e^{i\pi/2} \left[\cos\frac{\pi}{2} - i \sin\frac{\pi}{2} \left(\frac{\sigma_x + \sigma_z}{\sqrt{2}} \right) \right] \\
&= e^{i\pi/2} e^{-i\pi\left(\frac{\sigma_x + \sigma_z}{\sqrt{2}}\right)/2}
\end{aligned}$$

where $n_x = n_z = \frac{1}{\sqrt{2}}$.

Two-qubit gates are in $U(4)$

$U(4)$ is the group of unitary 4-by-4 matrices or operators. Similarly to the single-qubit gates, they can be expressed in terms of $SU(4)$

$$U(4) = U(1) \otimes SU(4)$$

where $U(1)$ is the group of complex numbers of the unit modulus, $e^{i\alpha}$, and $SU(4)$ is the group of unitary 4-by-4 matrices of the unit determinant.

$SU(4)$ Lie group and $su(4)$ algebra

The SU(4) group is 15-dimensional: $n^2 - 1 = 15$.

Each element of $SU(4)$ can be expressed as a complex exponential function of an element of the $su(4)$ algebra

$$e^{-i \sum_{ab} \theta_{ab} T_{ab}}$$

where T_{ab} are the generators of $su(4)$ algebra. They naturally split into two sets.

(i) Generators of local, single-qubit, operations

$$T_{a0} \;:\; T_{x0} = \frac{\sigma_x \otimes \hat{I}}{2},\;\; T_{y0} = \frac{\sigma_y \otimes \hat{I}}{2},\;\; T_{z0} = \frac{\sigma_z \otimes \hat{I}}{2}$$

$$T_{0a} \;:\; T_{0x} = \frac{\hat{I} \otimes \sigma_x}{2},\;\; T_{0y} = \frac{\hat{I} \otimes \sigma_y}{2},\;\; T_{0z} = \frac{\hat{I} \otimes \sigma_z}{2}$$

The generators from the first set commute with those of the second set. Each of these sets, generates a subgroup $SU(2)$, and thus together they generate the subgroup of all single qubit operations, over the first and second qubit, in the $SU(4)$ group:

$$SU(2) \otimes SU(2) \subset SU(4)$$

(ii) Generators of nonlocal operations

$$T_{ab} = \frac{\sigma_a \otimes \sigma_b}{2}$$

where $a, b = x, y, z$, giving the remaining nine generators:

$$T_{xx}, \;\; T_{xy}, \;\; T_{xz}, \;\; T_{yx}, \;\; T_{yy}, \;\; T_{yz}, \;\; T_{zx}, \;\; T_{zy}, \;\; T_{zz}$$

Physically these nonlocal generators originate from interaction between qubits. Their presence in the system Hamiltonian in general leads to time evolution that affects the state of both qubits and leads to changes of entanglement between both qubit.

The Lie brackets of all generators

$[T_{ij}, T_{kl}]$	T_{x0}	T_{y0}	T_{z0}	T_{0x}	T_{0y}	T_{0z}	T_{xx}	T_{xy}	T_{xz}	T_{yx}	T_{yy}	T_{yz}	T_{zx}	T_{zy}	T_{zz}
T_{x0}	0	T_{z0}	$-T_{y0}$	0	0	0	0	0	0	T_{zx}	T_{zy}	T_{zz}	$-T_{yx}$	$-T_{yy}$	$-T_{yz}$
T_{y0}	$-T_{z0}$	0	T_{x0}	0	0	0	$-T_{zx}$	$-T_{zy}$	$-T_{zz}$	0	0	0	T_{xx}	T_{xy}	T_{xz}
T_{z0}	T_{y0}	$-T_{x0}$	0	0	0	0	T_{yx}	T_{yy}	T_{yz}	$-T_{xx}$	$-T_{xy}$	$-T_{xz}$	0	0	0
T_{0x}	0	0	0	0	T_{0z}	$-T_{0y}$	0	T_{xz}	$-T_{xy}$	0	T_{yz}	$-T_{yy}$	0	T_{zz}	$-T_{zy}$
T_{0y}	0	0	0	$-T_{0z}$	0	T_{0x}	$-T_{xz}$	0	T_{xx}	$-T_{yz}$	0	T_{yx}	$-T_{zz}$	0	T_{zx}
T_{0y}	0	0	0	T_{0y}	$-T_{0x}$	0	T_{xy}	$-T_{xx}$	0	T_{yy}	$-T_{yx}$	0	T_{zy}	$-T_{zx}$	0
T_{xx}	0	T_{zx}	$-T_{yx}$	0	T_{xz}	$-T_{xy}$	0	T_{0z}	$-T_{0y}$	T_{z0}	0	0	$-T_{y0}$	0	0
T_{xy}	0	T_{zy}	$-T_{yy}$	$-T_{xz}$	0	T_{xx}	$-T_{0z}$	0	T_{0x}	0	T_{z0}	0	0	$-T_{y0}$	0
T_{xz}	0	T_{zz}	$-T_{yz}$	T_{xy}	$-T_{xx}$	0	T_{0y}	$-T_{0x}$	0	0	0	T_{z0}	0	0	$-T_{y0}$
T_{yx}	$-T_{zx}$	0	T_{xx}	0	T_{yz}	$-T_{yy}$	$-T_{z0}$	0	0	0	T_{0z}	$-T_{0y}$	T_{x0}	0	0
T_{yy}	$-T_{zy}$	0	T_{xy}	$-T_{yz}$	0	T_{yx}	0	$-T_{z0}$	0	$-T_{0z}$	0	T_{0x}	0	T_{x0}	0
T_{yz}	$-T_{zz}$	0	T_{xz}	T_{yy}	$-T_{yx}$	0	0	0	$-T_{z0}$	T_{0y}	$-T_{0x}$	0	0	0	T_{x0}
T_{zx}	T_{yx}	$-T_{xx}$	0	0	T_{zz}	$-T_{zy}$	T_{y0}	0	0	$-T_{x0}$	0	0	0	T_{0z}	$-T_{0y}$
T_{zy}	T_{yy}	$-T_{xy}$	0	$-T_{zz}$	0	T_{zx}	0	T_{y0}	0	0	$-T_{x0}$	0	$-T_{0z}$	0	T_{0x}
T_{zz}	T_{yz}	$-T_{xz}$	0	T_{zy}	$-T_{zx}$	0	0	0	T_{y0}	0	0	$-T_{x0}$	T_{0y}	$-T_{0x}$	0

Cartan decomposition of $SU(4)$

Every unitary operation $U \in SU(4)$ can be expressed using the Cartan decomposition

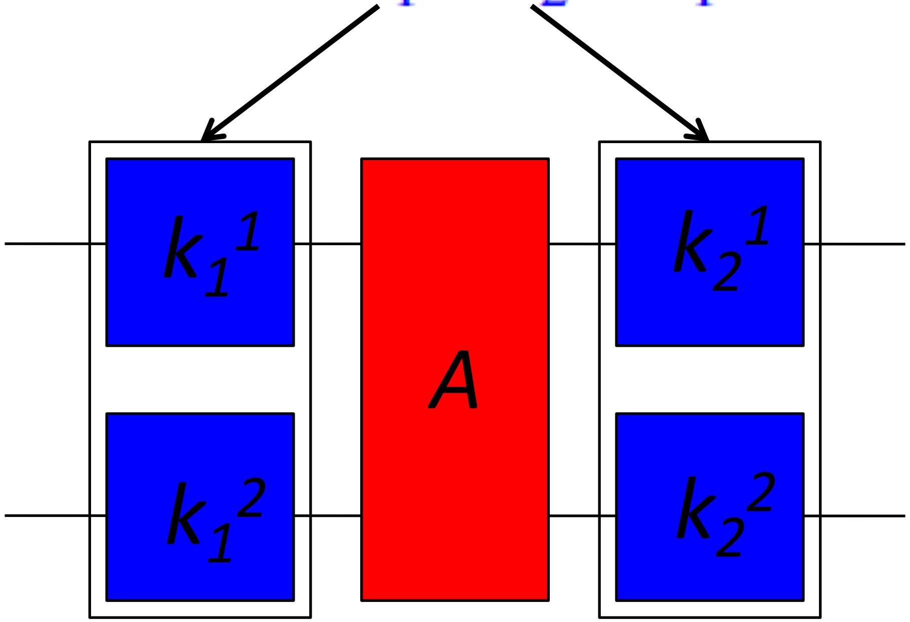
$$U \quad = \quad k_1 \; A \; k_2 = k_1 \; e^{\frac{i}{2}\left(c_1 \; \sigma_x^1 \sigma_x^2 + c_2 \; \sigma_y^1 \sigma_y^2 + c_3 \; \sigma_z^1 \sigma_z^2 \right)} \; k_2$$

where $k_1, k_2 \in SU(2) \otimes SU(2)$ are local gates. The part A embodies purely non-local content of the operation U and is generated by the maximal Abelian subalgebra of $SU(4)$ taht is spanned by the generators T_{xx}, T_{yy}, and T_{zz}.

The Cartan decomposition is indispensable in classification of the two-qubit operations according to their non-local content.

$$U \in SU(4)$$

$$U = k_1 \, A \, k_2 = k_1 \, e^{\frac{i}{2}\left(c_1 \, \sigma_x^1 \sigma_x^2 + c_2 \, \sigma_y^1 \sigma_y^2 + c_3 \, \sigma_z^1 \sigma_z^2 \right)} k_2$$



$$k_1, \, k_2 \in SU(2) \otimes SU(2)$$

Parameter counting:

6 + 3 + 6 = 15 = $4^2 - 1$

If two gates have the same *A* in the Cartan decomposition, they are locally equivalent:

$$U_1 = k_1 U_2 k_2$$

Local equivalence classes and the Weyl chamber

The Cartan decomposition contains extra symmetries, including interchanges of c_1 c_2 and c_3 with and without sign flips. These can be removed using theory of local invariants and Weyl reflection symmetries. This allows us to classify the two-qubit operations in terms of their local equivalence classes.

We say the operations U_1 and U_2 are **locally equivalent** if U_1 and U_2 are related by local, i.e. single qubit operations: $U_1 = k_1 U_2 k_2$.

The set of all operations that are locally equivalent forms **local equivalence class**.

The set of all local equivalence classes forms the coset

$$SU(4)/SU(2) \otimes SU(2).$$

Local invariants (Makhlin 2002, Zhang et al. 2003)
The local equivalence classes of two-qubit operations are most conveniently defined using **local invariants** which uniquely characterize two-qubit operations up to an arbitrary single qubit transformations $k_1, k_2 \in SU(2) \otimes SU(2)$.

Unitary transformation of any $U \in SU(4)$ into the Bell basis

$$U_B = U_Q^\dagger U U_Q = U_Q^\dagger k_1 U_Q U_Q^\dagger A U_Q U_Q^\dagger k_2 U_Q = O_1 F O_2,$$

$$\text{where } U_Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{pmatrix}$$

changes k_1 and k_2 into orthogonal matrices O_1 and O_2 respectively, with the property $O^T O = \hat{1}$, and transforms the non-local factor of the Cartan decomposition A into a diagonal matrix F.

Constructing the Makhlin matrix

$$m = U_B^T U_B = O_2^T F O_1^T O_1 F O_2 = O_2^T F^2 O_2$$

eliminates one of the local factors in the Cartan decomposition of U and shows that O_2 diagonalizes the Makhlin matrix, indeed $F^2 = O_2 m O_2^T$.

From the corresponding characteristic equation, we could derive the local invariants

$$\begin{aligned} g_1 &= \frac{1}{16} Re\left[\mathrm{tr}^2(m)\right] \\ g_2 &= \frac{1}{16} Im\left[\mathrm{tr}^2(m)\right] \\ g_3 &= \frac{1}{4}\left[\mathrm{tr}^2(m) - \mathrm{tr}\,(m^2)\right]. \end{aligned}$$

Since the trace of a matrix is invariant w.r.t. a unitary transformation of the matrix, the effect of the remaining local factor of the Cartan decomposition k_2 has been eliminated, and the invariants indeed depend only on the matrix A.

For general two-qubit unitary matrices $U \in U(4)$ whose determinants are any complex number of unit modulus, we can define the local invariants as

$$
\begin{aligned}
g_1 &= \frac{Re\left[\operatorname{tr}^2(m)\right]}{16\det(U)} \\
g_2 &= \frac{Im\left[\operatorname{tr}^2(m)\right]}{16\det(U)} \\
g_3 &= \frac{\left[\operatorname{tr}^2(m) - \operatorname{tr}(m^2)\right]}{4\det(U)}.
\end{aligned}
$$

where the division by $\det(U)$ eliminates the dependence on a global phase of U.

Example: Selected elements of the local equivalence class $[CNOT]$

$$U_{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad U_{CPHASE} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad U_Q = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{pmatrix}$$

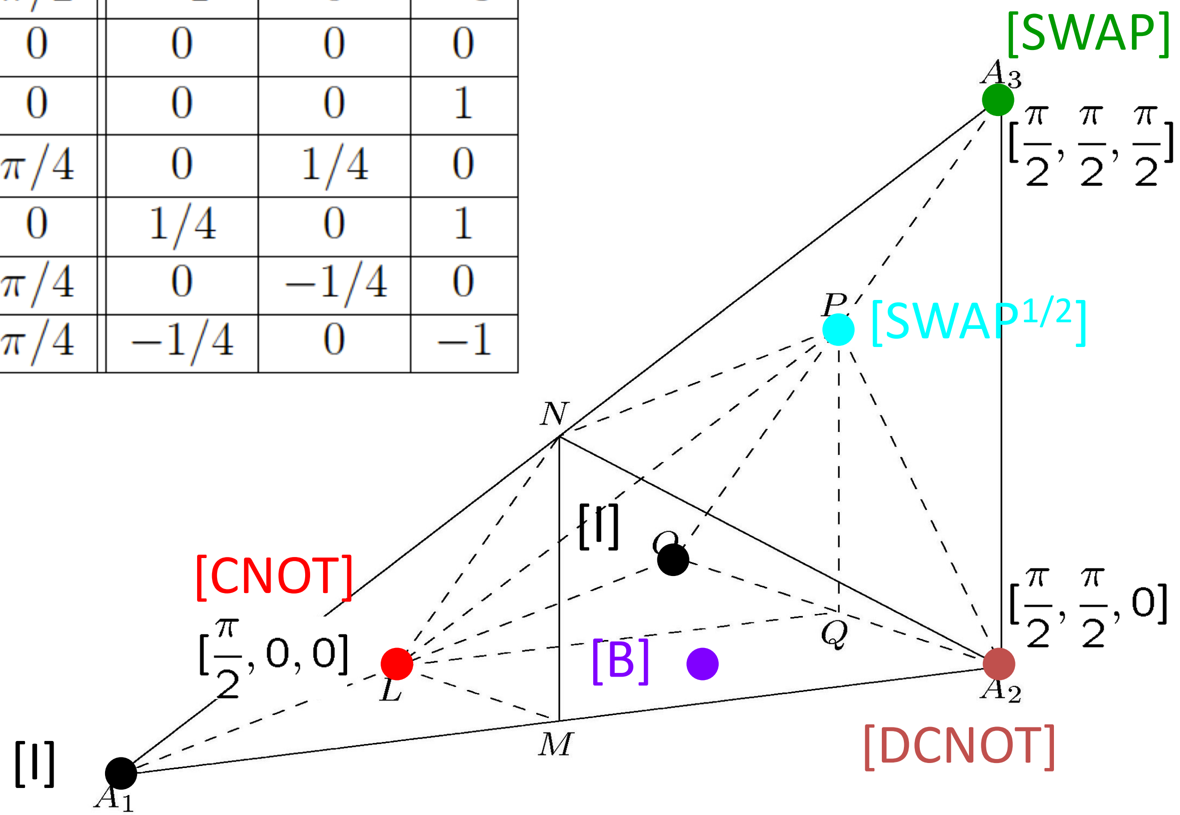
The local invariants of all these matrices from the group $U(4)$ are

$$\begin{aligned} g_1 &= \frac{Re\left[\mathrm{tr}^2(m)\right]}{16\det(U)} = 0, \\ g_2 &= \frac{Im\left[\mathrm{tr}^2(m)\right]}{16\det(U)} = 0, \\ g_3 &= \frac{\left[\mathrm{tr}^2(m) - \mathrm{tr}\,(m^2)\right]}{4\det(U)} = 1, \end{aligned}$$

where $\det(U) = -1$ for all the matrices in the example.

Weyl chamber

point (gate)	c_1	c_2	c_3	g_1	g_2	g_3
O, A_1 ([$\mathbb{1}$])	0, π	0	0	1	0	3
A_2 ([DCNOT])	$\pi/2$	$\pi/2$	0	0	0	-1
A_3 ([SWAP])	$\pi/2$	$\pi/2$	$\pi/2$	-1	0	-3
B ([B-Gate])	$\pi/2$	$\pi/4$	0	0	0	0
L ([CNOT])	$\pi/2$	0	0	0	0	1
P ([$\sqrt{\text{SWAP}}$])	$\pi/4$	$\pi/4$	$\pi/4$	0	$1/4$	0
Q, M	$\pi/4$, $3\pi/4$	$\pi/4$	0	$1/4$	0	1
N	$3\pi/4$	$\pi/4$	$\pi/4$	0	$-1/4$	0
R	$\pi/2$	$\pi/4$	$\pi/4$	$-1/4$	0	-1



Universal set of quantum computing operations

Universal set of quantum computing gates is the set of operations that allows us to implement any computable function, i.e. any quantum computation algorithm or any unitary operation over n qubits, on a quantum computer.

Universality in quantum computation means the ability to generate an arbitrary element of the group of special unitary operations over n qubits, that is, an arbitrary element of the group $SU(2^n)$.

Solovay-Kitaev theorem

Given a set of gates that is dense in $SU(2^n)$ and closed under hermitian conjugation, any gate $U \in SU(2^n)$ can be approximated to an accuracy ϵ with a sequence of poly[log(1/ϵ)] gates from the set.

Universal quantum computation can be realized by a circuit of two-qubit and single-qubit gates from a universal set.

Examples of universal sets:

(i) Continuous: $SU(2)$ over any qubit, and $CNOT$ on any pair of qubits.
(ii) Discrete (approximation): Hadamard, phase flip $\hat{Z}$, $\hat{T}$, $CNOT$.