Quantum Theory: Unitary Dynamics

- Quantum dynamics should map quantum states to quantum states, which means they should preserve the 2-norm. These are called orthogonal transformations (over \mathbb{R}) and unitary transformations (over \mathbb{C}).
- Orthogonal and unitary transformations are defined as those linear transformations that preserve inner products. Given a linear operator U on a vector space \mathcal{V} , there is a corresponding adjoint operator U^{\dagger} which acts on the dual space, so that the co-vector of $U|\psi\rangle$ is $\langle \psi|U^{\dagger}$. In finite dimensional spaces, the matrix corresponding to U^{\dagger} is the transpose conjugate of U.
- The property of preserving inner products means $\langle \phi | U^{\dagger} U | \psi \rangle = \langle \phi | \psi \rangle$ for all $|\psi \rangle, |\phi \rangle$, which implies

$$U^{\dagger}U = I$$

This equation implies $U^{-1} = U^{\dagger}$, in other words unitary evolution is always invertible.

Quantum Theory: Unitary Dynamics

An immediate intuition for unitary transformations can be gained by the fact that they preserve inner products (and hence the 2-norm). They preserve Euclidean distance, and are therefore **rotations**.

Invertibility is just the tip of the iceberg. This property implies that unitary transformations (or unitary matrices) form a group under multiplication. A continuous group that is also a compact manifold. The group U(d) of unitary transformations on a d-dimensional space is a classically studied **Lie Group**.

Consider a continuous one-parameter group of unitary transformations $\{U(t) : t \in \mathbb{R}\}$ satisfying

$$U(t)U(t') = U(t+t')$$

Representing the homogeneous time-evolution of a quantum syste. Stone's theorem says that

$$U(t) = e^{itA}$$

For some self-adjoint operator A (self-adjoint means $A = A^{\dagger}$, which is equivalently called a Hermitian operator i.e. an observable...)

Quantum Theory: Unitary Dynamics

More generally, the instantaneous unitary time evolution of a quantum state $|\psi(t)\rangle$ is generated by a (potentially time-dependent) Hermitian operator H(t), yielding the famous Schrodinger equation:

$$i\frac{d}{dt}|\psi(t)
angle = H(t)|\psi(t)
angle$$

The operator H(t) is called the **Hamiltonian**, and it turns out to correspond to an observable of fundamental importance called the **energy** of the quantum system.

The point of "energy" is that it is conserved. It is invariant under time relations. In physics, symmetries correspond to conserved quantities, and energy is the conserved quantity corresponding to time translation symmetry.

This relationship of energy and time translation symmetry is what lies behind the Schrodinger equation. A beautiful treatment can be found in Sakurai's Graduate Physics QM book. For us it is too much of a tangent and so we will accept it as the **axiom of dynamics**.

Quantum Computer: just like the stochastic gate model, but now all gates (P, W, R, Q) are unitary.



Axioms of QM

- Axiom of states. States are rays in Hilbert space, or unit vectors in the 2-norm.
- Axiom of composition. The state of a composite system is a vector in the Hilbert space given by the tensor product of the Hilbert spaces of the component subsystems.
- Axiom of observables. An observable is a set of events that are associated with real values, formally represented as a Hermitian operator. Expectation values are given by inner products with this operator. (The dimension *N* of the Hilbert space of states is the number of events associated to each observable.)
- Axiom of Measurement. Measuring a particular observable on a particular state returns a value associated with a particular event, after which the state is updated to the vector corresponding to that event.
- Axiom of Dynamics. Quantum time-evolution is a unitary transformation. This evolution is generated at each instant in time by a Hermitian operator called the Hamiltonian, which is the observable corresponding to energy, according to the Schrodinger equation.

The axiomatic description of QM given so far allows us to perform many calculations: given an explicit vector / matrix description of a state, unitary, and observable we can time-evolve the state with the unitary, and compute the expectation of the observable in the resulting state.

This level of description suffices to understand the abstract operation of a quantum computer: the initial state is given, the unitary evolutions are given (as allowed combinations of local unitary gates), and the final state is sampled in the computational basis. (also note that incompatible observables / event spaces are not needed to describe the quantum computation)



Quantum Information Science deals almost entirely within this abstract framework, because it assumes that (within some general rules) we can engineer these basic building blocks (states, unitaries, etc). But how is this done, how does QI manifest in physical systems?

"Mike and Ike" on Hamiltonians

"In general figuring out the Hamiltonian needed to describe a particular physical system is a very difficult problem – much of twentieth century physics has been concerned with this problem – which requires substantial input from experiment in order to be answered. From our point of The postulates of quantum mechanics this is a problem of detail to be addressed by physical theories built within the framework of quantum mechanics – what Hamiltonian do we need to describe atoms in such-and-such a configuration – and is not a question that needs to be addressed by the theory of quantum mechanics itself

Most of the time in our discussion of quantum computation and quantum information we won't need to discuss Hamiltonians, and when we do, we will usually just posit that some matrix is the Hamiltonian as a starting point, and proceed from there, without attempting to justify the use of that Hamiltonian."

- Nielson and Chuang, page 82.

The derivation or explanation of the physical origin of the unitaries that describe the evolution of a QM system involves several ingredients.

Step 1. Identify the relevant physical observables that describe the system.

These may be position and momentum for particles moving in space, or charge and magnetic flux in electrical circuits, or directional components of angular momentum / particle spin.



Step 2. Determine the representation of the physical observables as linear operators / matrices.

Given a single observable $A = \sum_i a_i |a_i\rangle \langle a_i|$, we can choose the associated basis of events to be the standard basis of unit vectors. Together with the real values associated with those events, this allows us to construct a representation of the observable as a diagonal matrix:

Now given a second observable $B = \sum_i b_i |b_i\rangle \langle b_i|$, associated with some incompatible basis of events, how to represent B as a matrix?

$$A = \begin{bmatrix} a_0 & 0 & \dots \\ \vdots & \ddots & \\ 0 & & a_{N-1} \end{bmatrix}$$

Representation theory is an area of mathematics that is concerned with representing abstract groups or algebras in terms of matrices. In short, to determine the matrix representation of B in the basis in which A is diagonal, it will suffice for us to know the **algebraic relations** between A and B (and possibly other observables that enter into the description of this system)

Step 2. Determine the representation of the physical observables as linear operators / matrices.

A complete set of observables for a system forms a C*-algebra. This refers to closure under properties including addition, multiplication, multiplication by scalars, and taking adjoints.

The representations we seek are determined by algebraic relations called commutators:

$$[A,B] = AB - BA = C$$

There is a direct prescription to determine the commutators for a set of physical observables which was put forth by Dirac, called "canonical quantization", which builds on Hamilton's classical mechanics.

Step 2. Determine the representation of the physical observables as linear operators / matrices.

In classical mechanics, observables A,B are real-valued functions of generalized coordinates q, p (which can be thought of as generalizations of position and momentum).

The **Poisson bracket**
$$\{A, B\}_{\mathcal{P}}$$
 of A, B is defined by: $\{A, B\}_{\mathcal{P}} = \sum_{i=1}^{N} \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i}$

Dirac's brilliant prescription of canonical quantization is to promote Poisson brackets to commutators:

$$[A,B] = i\{A,B\}_{\mathcal{P}}$$

We won't get into the mathematical justification (based on the "symplectic structure" of the classical Hamiltonians equations), but if you like this prescription works because of the **correspondence principle**.

Step 3. Find the Hamiltonian by expressing the energy in terms of physical observables.

Once the relevant physical variables describing the system have been identified, the next step is to express the collective energy of the system in terms of observables corresponding to the constituent parts.

In some cases this is done from first principles, by porting known energy functions from classical physics:

 $H = p^2 + q^2$

Harmonic oscillator (universal description of small oscillations)

Magnetic field B

 $H = -\vec{\mu} \cdot \vec{B}$

magnetic dipole (e.g. rotating charged particle) in an external magnetic field

 $\vec{\mu}$ = magnetic dipole moment

Step 3. Find the Hamiltonian by expressing the energy in terms of physical observables.

In other cases the Hamiltonian may be an **effective** description that one finds by beginning with a complicated first principles description and making approximations.

$$H = p^2 + q^2$$

Electrical circuits are an effective description, with observables like current, charge, voltage, and magnetic flux.





$$H = -\vec{S_1} \cdot \vec{S_2}$$

Magnetism in matter is explained by an effective theory of spinspin interactions.

In some cases, we may only have a **phenomenological** description that is inferred from experiment without understanding the underlying physics, but this can still be used to make predictions.

Step 4. Determine the time-evolution by solving the Schrodinger equation.

Once H is expressed in terms of physical observables which have known matrix representations, the matrix representation of H itself is known, and the Schrodinger equation / IVP:

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$
, $|\psi(t=0)\rangle = |\psi^{\text{init}}\rangle$

becomes a system of N coupled linear differential equations, in which time t is the independent variable and the components of the wave function $(\psi_0(t), ..., \psi_{N-1}(t))$ are the unknown functions.

If H is time-independent H(t) = H then the solution to the initial value problem is:

$$|\psi(t)\rangle = e^{-itH}|\psi^{\text{init}}\rangle$$

Step 4. Determine the time-evolution by solving the Schrodinger equation.

This solution in terms of the matrix exponential can be computed with the eigendecomposition:

$$H = \sum_{i=1}^{N} E_i |E_i\rangle \langle E_i| \implies e^{-itH} = \sum_{i=1}^{N} e^{-itE_i} |E_i\rangle \langle E_i|$$
$$|\psi(t)\rangle = e^{-itH} |\psi^{\text{init}}\rangle \implies |\psi(t)\rangle = \sum_{i=1}^{N} e^{-itE_i} \langle E_i |\psi^{\text{init}}\rangle |E_i\rangle$$

The eigendecomposition of an N x N Hermitian matrix can be computed in time $O(N^3)$ by Gaussian elimination, so this is relatively efficient in the dimension of the system.

The eigenstates of H correspond to events with a definite energy, which may be measurable, so diagonalizing H has additional purpose besides time evolution.

The Schrodinger equation relates energy *H* to rate of change $\frac{\partial}{\partial t}$ of a state.

This relation of energy and time grew in part from the 19th century connection between time translation symmetry and an associated conserved quantity (which we call energy), which culminated in the theory of relativity (which sees energy as the time-analog of spatial momentum).

More directly, Schrodinger's equation followed from the Planck-Einstein relation between the energy *E* of a photon and its angular frequency ω :

$$E = \hbar \omega$$
 , $\hbar = 1.0545718 \times 10^{-34}$ meter²kilogram/second

Schrodinger's equation is really: $i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$ and the Hamiltonians also have \hbar 's

The point is that \hbar is a constant that reflects the scale of quantum effects, relative to our choice of fundamental units. If our fundamental units are macroscopic quantities like meters, kilograms, and seconds, then \hbar is small. But to simplify formulas while doing theory, we always take $\hbar = 1$.

Step 1. Identify the relevant physical observables that describe the system.

Step 2. Determine the representation of the physical observables as linear operators / matrices.

Step 3. Find the Hamiltonian by expressing the energy in terms of physical observables.

Step 4. Determine the time-evolution by solving the Schrodinger equation.

We now have an axiomatic description of QM, together with 4 step process for describing physical systems quantum mechanically. We are now ready to explore the consequences!



"I think I can safely say that nobody understands quantum mechanics...."

Richard Feynman



"I think I can safely say that nobody understands quantum mechanics...." "If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet."



Niels Bohr

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"...in mathematics you don't understand things, you just get used to them."



John von Neumann



Richard Feynman

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Niels Bohr



"QM makes perfect sense as an L2 generalization of probability theory, to include amplitude interference and incompatible sets of events." "...in mathematics you don't understand things, you just get used to them."



John von Neumann

Arrogant 21st century person

The simplest quantum system is 2-dimensional, it is called a "qubit" which is short for quantum bit.

$$\begin{split} |\psi\rangle &= \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad, \quad \alpha,\beta \in \mathbb{C} \ , \ |\alpha|^2 + |\beta|^2 = 1 \end{split}$$
 The standard basis vectors are defined to be
$$\ |0\rangle &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad, |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Therefore arbitrary states may be expressed as
$$|\psi
angle=egin{bmatrix}lpha\\eta\end{bmatrix}=lpha|0
angle+eta|1
angle$$

Following our four step process for populating the theory with physical content, the next question is: what are the physical observables for a qubit?



The Stern-Gerlach experiment suggests that we can measure the quantum spin of the electron along any choice of spatial direction, and obtain two possible measurement outcomes. For each spatial axis \hat{r} we can measure the spin along \hat{r} and obtain one of two possible outcomes.

Classically, spin is a 3-vector $\vec{S} = S_x \hat{x} + S_y \hat{y} + S_z \hat{z}$, so the three observables $\{S_x, S_y, S_z\}$ form a basis for the full set of observables. Each measurements in the SG experiment has two outcomes, so we are looking for a 2 x 2 Hermitian matrix to represent each of $\{S_x, S_y, S_z\}$.

It turns out that the set of Poisson brackets $\{S_x, S_y, S_z\}$ (and hence commutators of these operators after canonical quantization) is closed. The commutators are given by

$$[S_x, S_y] = 2iS_z$$
, $[S_y, S_z] = 2iS_x$, $[S_z, S_x] = 2iS_y$

These **commutator relations** are known to Mathematicians as defining a basis for the **Lie algebra for SU(2)**. The important point is that the representation theory for this algebra is well understood.

We will use these operators $\{S_x, S_y, S_z\}$ so frequently that we will simply call them $\{X, Y, Z\}$ (note that sometimes texts define $S_x = (\hbar/2)X$ but we are relatively unconcerned about constants.)

$$[X, Y] = 2iZ$$
 , $[Y, Z] = 2iX$, $[Z, X] = 2iY$

A 2 x 2 representation of the algebra of observables satisfying these commutation relations takes:

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

These **Pauli matrices** are the fundamental observables associated to qubits. Commit these commutator relations and matrix representations to memory ("minus i up high").

We first consider the Pauli matrix that is easiest to diagonalize: $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

The eigenvectors of this matrix are
$$\ \ket{0}=egin{bmatrix}1\\0\end{bmatrix}$$
 , $\ket{1}=egin{bmatrix}0\\1\end{bmatrix}$, and hence satisfy

$$Z|0\rangle = |0\rangle \quad , \quad Z|1\rangle = -|1\rangle$$

Therefore (by choice of convention) the computational basis corresponds to the eigenstates of Pauli Z. For an arbitrary state, the expectation value of the spin along the Z direction is

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \implies \langle \psi | Z | \psi \rangle = |\alpha|^2 - |\beta|^2$$

The next Pauli matrix to consider is Pauli X: $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

The eigenvectors of this matrix are named $|+\rangle, |-\rangle$ and are given by

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\1 \end{bmatrix} \quad , |-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\-1 \end{bmatrix}$$

These satisfy ~X|+
angle=|+
angle~~,~~X|angle=-|angle . We can relate these to the computational basis:

$$|+\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \qquad |0\rangle = \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle) \\ |-\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \qquad |1\rangle = \frac{1}{\sqrt{2}} (|+\rangle - |-\rangle)$$

The last (and least) Pauli matrix is $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

The eigenvectors of this matrix don't have common names, but are sometimes called

$$|i\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\i \end{bmatrix} \quad , |-i\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\-i \end{bmatrix}$$

Which again are the +/- 1 eigenstates. The reason that Y is often neglected is that

$$Y = iXZ$$

So we can account for the action of Y by a combination of X, Z, and a global phase. In all seriousness, Pauli Y is essential for completeness, but since two bases of incompatible events often suffice to describe quantum information processing, we will focus much more on X, Z.



Bloch Sphere:

$$|\psi(\theta,\phi)\rangle = \cos\left(\frac{\theta}{2}\right)|0
angle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1
angle$$

The point is that single qubit states can be
 specified by two real angles, θ, φ, which establish a correspondence between 2D complex unit vectors, and 3D real unit vectors.

Memorizing the Bloch sphere will let you more quickly see the expectations of $\{X, Y, Z\}$ for states written in components. But this geometric picture does not generalize well to higher dimensions (multiple qubits) and so we will not emphasize it.

Each Pauli operator has eigenvalues $\{1, -1\}$, and so the Paulis are **traceless**:

$$\operatorname{tr}(X) = \operatorname{tr}(Y) = \operatorname{tr}(Z) = 1 - 1 = 0$$

If we include the identity operator, then $\{I, X, Y, Z\}$ form a basis for 2 x 2 Hermitian matrices.

$$A = \alpha_I I + \alpha_x X + \alpha_y Y + \alpha_z Z$$

How do you prove this?

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How do you prove this?
$$\begin{bmatrix} a \\ b^{\dagger} \end{bmatrix}$$

Hermitian matrix has 4 real parameters. ($a = a^{\dagger}$, $c = c^{\dagger}$) 2 x 2 matrices isomorphic to 1 x 4 vectors.

Frobenius Inner Product: $\langle A,B
angle_{
m F}={
m tr}\left(A^{\dagger}B
ight)$

Dropping the identity component, we can represent all traceless 2 x 2 Hermitian matrices by

$$A = \alpha_x X + \alpha_y Y + \alpha_z Z = \boldsymbol{\alpha} \cdot \boldsymbol{\sigma} \quad , \quad \boldsymbol{\alpha} = (\alpha_x, \alpha_y, \alpha_z) \; , \; \boldsymbol{\sigma} = (X, Y, Z)$$

Since every 2 x 2 Unitary matrix has the form $U = e^{iA}$ for Hermitian A, and the identity component would only generate an irrelevant global phase, we can parameterize all 2 x 2 unitary matrices:

$$U_{\alpha} = e^{i\alpha \cdot \sigma}$$

We have already encountered the first examples of single qubit unitaries: the Pauli matrices! They do double-duty as Hermitian matrices that happen to be unitary. If A is Hermitian and unitary, then

$$A = A^{\dagger}$$
 and $A^{\dagger}A = I \implies A^{\dagger}A = A^2 = I$

Which is true of the Paulis, $X^2 = Y^2 = Z^2 = I$. Memorize the action of these unitaries:

Pauli X is a "bit flip" or NOT gate:		
$X 0\rangle = 1\rangle$,	$X 1\rangle = 0\rangle$
$X +\rangle = +\rangle$,	$X -\rangle = - -\rangle$
)

Pauli Z is a "Phase flip":Z|0
angle=|0
angle~,~~Z|1
angle=-|1
angleZ|+
angle=|angle~,~~Z|angle=|+
angle

The next class of unitaries we may consider are rotations around the Z axis, called phase shift gates:

$$U_{\theta} = e^{i\theta Z} = \begin{bmatrix} e^{i\theta} & 0\\ 0 & e^{-i\theta} \end{bmatrix}$$

Note that
$$Z^{1/k} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/k} \end{bmatrix}$$

The next class of unitaries are rotations around the Y axis, which rotate vectors in the X/Z plane:

$$U_{\theta} = e^{i\theta Y} = \begin{bmatrix} \cos\theta & -\sin\theta\\ \sin\theta & \cos\theta \end{bmatrix}$$

Unitary matrices with real entries are called orthogonal matrices. The rotation matrices above commonly appear in linear algebra as rotations of vectors in \mathbb{R}^2 .

If we combine a $\pi/4$ rotation in the XZ-plane, followed by a Z rotation we obtain

$$H = Z \cdot e^{i\frac{\pi}{4}Y} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1\\ 1 & -1 \end{bmatrix}$$

This unitary transformation is called a Hadamard gate, hence the use of the symbol H (fortunately H is also Hermitian, so $H^2 = I$ since H is Hermitian and unitary).

The Hadamard gate is extremely important because it is the change of basis between Z and X. Memorize:

$$\begin{array}{l} H|+\rangle = |0\rangle \\ H|-\rangle = |1\rangle \end{array} \hspace{1.5cm} H|0\rangle = |+\rangle \\ H|1\rangle = |-\rangle \end{array}$$

From the matrix form $A = \sum_{i,j} A_{ij} |i\rangle \langle j|$ it is clear that if kets transform like $|\psi\rangle \rightarrow U |\psi\rangle$ then $A \rightarrow U A U^{\dagger}$ (change of basis for operators)

The Hadamard gate changes between the +/- basis and the 0/1 basis, so its no surprise that

$$X = H \cdot Z \cdot H \quad , \quad Z = H \cdot X \cdot H$$

Some other operator transformations worth memorizing include:

$$X = -Z \cdot X \cdot Z \quad , \quad Z = -X \cdot Z \cdot X$$

So conjugating X with Z yields –X, and conjugating Z with X yields –Z.

Notice that we have some unitaries that map Pauli operators to Pauli operators: this includes the Hadamard gate, and also the Paulis themselves.

Let $\mathcal{P} = \{I, X, Y, Z\}$ be the Pauli group. What unitaries U have the property that

 $\sigma \in \mathcal{P} \implies U \sigma U^{\dagger} \in \mathcal{P}$

So far we have Hadamard, and $\{X, Y, Z\}$. Are there any others?

Notice that we have some unitaries that map Pauli operators to Pauli operators: this includes the Hadamard gate, and also the Paulis themselves.

Let $\mathcal{P} = \{I, X, Y, Z\}$ be the Pauli group. What unitaries U have the property that

 $\sigma \in \mathcal{P} \implies U \sigma U^{\dagger} \in \mathcal{P}$

So far we have Hadamard, and $\{X, Y, Z\}$. Are there any others? If there is a unitary matrix that takes X to Z, then there must be another taking X to Y, by symmetry.

$$p = \sqrt{Z} = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$$
, $p \cdot X \cdot p = Y$

The set of unitaries that map Pauli operators to Pauli operators is called the **Clifford Group**. Clifford unitary transformations are of interest because they map any string of Paulis as input to a string of Paulis as output, in an efficiently computable way. <u>The single qubit Clifford Group is generated by H and p.</u>

Qubits: Observables and Unitaries

- Qubits are the simplest quantum systems, representing by vectors in the Hilbert space \mathbb{C}^2
- Whether by considering classical angular momentum and applying canonical quantization, or by choosing a convenient basis for the set of Hermitian matrices, we arrive at the Pauli matrices as qubit observables.

• The Pauli matrices are traceless, Hermitian and unitary (and hence are their own matrix inverse). According to the Bloch sphere representation they measure spin along the cartesian directions X,Y,Z.

• We formed several 2 x 2 single qubit unitary matrices by exponentiating linear combinations of Pauli matrices. Of particular interest are the Clifford transformations, which map Paulis to Paulis.