# Quantum Computing
# 3 - Quantum Mechanics

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# The Postulates of Quantum Mechanics

We have reviewed the mathematics (complex linear algebra) necessary to understand quantum mechanics. We will now see how the *physics* of quantum mechanics fits into this mathematical framework.

We are really defining the *structure* of a quantum theory. All physical theories based on quantum mechanics share this common structure. Later in the course, we will see how this mathematical structure is realized for realistic systems. For now, we will use our simple example of the spin-1/2 particle to illustrate these ideas.

# Postulate 1: State space

Every physical system has an associated Hilbert space H of some dimension D, known as the state space of that system; and the system is completely described by its state vector, which is a unit vector in the state space.

If we choose a particular basis for the Hilbert space $|j\rangle$, $j = 1, \ldots, D$, a state can be written in the form

$$|\psi\rangle = \sum_{j=1}^{D} \alpha_j |j\rangle, \quad \text{where} \sum_j |\alpha_j|^2 = 1.$$

In the case of spin-1/2, we can write any state in terms of the basis "spin up" and "spin down" along the Z axis:

$$|\psi\rangle = \alpha_1 |\uparrow_Z\rangle + \alpha_2 |\downarrow_Z\rangle.$$

The overall phase of the state has no physical meaning, so $|\psi\rangle$ and $e^{i\vartheta}|\psi\rangle$ represent the same physical state.

The choice of basis relates to possible measurements of the system. As we will see, each basis is associated with a particular measurement (or group of compatible measurements), and each basis vector with a particular measurement outcome.

For spin-1/2 each basis is associated with a particular direction in space along which the component of the spin could be measured. So $\{|\uparrow_Z\rangle, |\downarrow_Z\rangle\}$ is associated with measurement of the component of spin along the *Z* axis, with the basis vectors corresponding to spin up or down.

Similarly, the bases $\{|\uparrow_X\rangle, |\downarrow_X\rangle\}$ and $\{|\uparrow_Y\rangle, |\downarrow_Y\rangle\}$ represent other possible measurements.

# Postulate 2: Unitary time evolution

The time-evolution of a closed system is described by a unitary transformation,

$$|\psi(t_2)\rangle = U(t_2, t_1)\,|\psi(t_1)\rangle,$$

where U is independent of the initial state.

In fact, the time-evolution of the state is given by the Schrödinger equation

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

where $H(t)$ is an Hermitian operator (the *Hamiltonian*) that describes the *energy* of the system. How does this relate to unitary transformations?

This is easiest to see if H is a fixed operator (i.e., constant in time). In that case, a solution to Schrödinger's equation is

$$|\psi(t_2)\rangle = \exp(-i\hat{H}(t_2 - t_1)/\hbar)|\psi(t_1)\rangle.$$

The operator $-H(t_2 - t_1)/hbar$ is Hermitian, so the operator

$$\hat{U}(t_2, t_1) = \exp(-i\hat{H}(t_2 - t_1)/\hbar)$$

is unitary, as asserted.

Suppose there is a uniform magnetic field in the $Z$ direction. Then states with spin up and down along the $Z$ axis have different energies. This is represented by a Hamiltonian

$$\hat{H} = \begin{pmatrix} E_0 & 0 \\ 0 & -E_0 \end{pmatrix} \equiv E_0\hat{Z},$$

where $E_0$ is proportional to the strength of the magnetic field. If $|\psi\rangle = \alpha|\uparrow_Z\rangle + \beta|\downarrow_Z\rangle$ at $t = 0$, then

$$|\psi(t)\rangle = \alpha e^{-iE_0t/\hbar}|\uparrow_Z\rangle + \beta e^{iE_0t/\hbar}|\downarrow_Z\rangle.$$

This type of evolution is equivalent to a steady rotation about the $Z$ axis, called *precession*.

# Examples

**EXAMPLE 2.1** Let us consider a time-independent Hamiltonian

$$H = -\frac{\hbar}{2}\omega\sigma_x. \tag{2.8}$$

Suppose the system is in the eigenstate of $\sigma_z$ with the eigenvalue $+1$ at time $t = 0$;

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The wave function $|\psi(t)\rangle$ $(t > 0)$ is then found from Eq. (2.5) to be

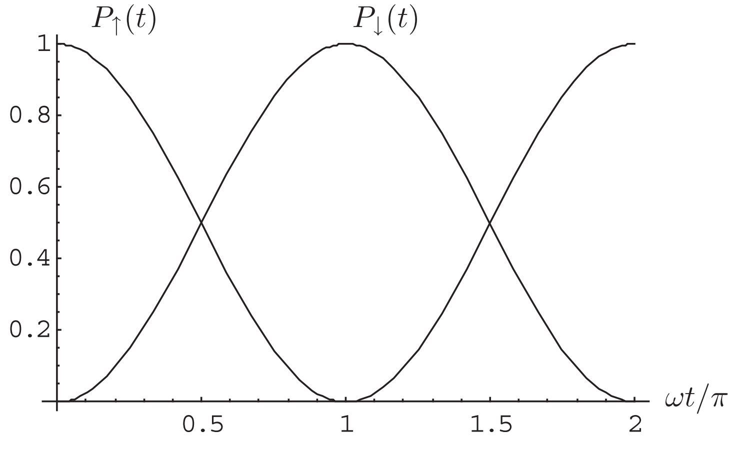
$$|\psi(t)\rangle = \exp\left(i\frac{\omega}{2}\sigma_x t\right)|\psi(0)\rangle. \tag{2.9}$$

The matrix exponential function in this equation is evaluated with the help of Eq. (1.44) and we find

$$|\psi(t)\rangle = \begin{pmatrix} \cos\omega t/2 & i\sin\omega t/2 \\ i\sin\omega t/2 & \cos\omega t/2 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\omega t/2 \\ i\sin\omega t/2 \end{pmatrix}. \tag{2.10}$$

Suppose we measure the observable $\sigma_z$. Note that $|\psi(t)\rangle$ is expanded in terms of the eigenvectors of $\sigma_z$ as

$$|\psi(t)\rangle = \cos\frac{\omega}{2}t|\sigma_z = +1\rangle + i\sin\frac{\omega}{2}t|\sigma_z = -1\rangle.$$




The state oscillates among the two eigenstates. Why? What should happen to not have the oscillation? What are the probabilities of outcomes of measurements?

Next let us take the initial state

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

which is an eigenvector of $\sigma_x$ (and hence the Hamiltonian) with the eigenvalue $+1$. We find $|\psi(t)\rangle$ in this case as

$$|\psi(t)\rangle = \begin{pmatrix} \cos\omega t/2 & i\sin\omega t/2 \\ i\sin\omega t/2 & \cos\omega t/2 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{e^{i\omega t/2}}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{2.11}$$

Therefore the state remains in its initial state at an arbitrary $t > 0$. This is an expected result since the system at $t = 0$ is an eigenstate of the Hamiltonian.

**EXERCISE 2.2** Let us consider a Hamiltonian

$$H = -\frac{\hbar}{2}\omega\sigma_y. \tag{2.12}$$

Suppose the initial state of the system is

$$|\psi(0)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.13}$$

(1) Find the wave function $|\psi(t)\rangle$ at later time $t > 0$.
(2) Find the probability for the system to have the outcome $+1$ upon measurement of $\sigma_z$ at $t > 0$.
(3) Find the probability for the system to have the outcome $+1$ upon measurement of $\sigma_x$ at $t > 0$.

Now let us formulate Example 2.1 and Exercise 2.2 in the most general form. Consider a Hamiltonian

$$H = -\frac{\hbar}{2}\omega \hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}, \tag{2.14}$$

where $\hat{\boldsymbol{n}}$ is a unit vector in $\mathbb{R}^3$. The time-evolution operator is readily obtained, by making use of the result of Proposition 1.2, as

$$U(t) = \exp(-iHt/\hbar) = \cos\frac{\omega}{2}t\ I + i(\hat{\boldsymbol{n}} \cdot \boldsymbol{\sigma}) \sin\frac{\omega}{2}t. \tag{2.15}$$

Suppose the initial state is

$$|\psi(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

for example. Then we find

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = \begin{pmatrix} \cos(\omega t/2) + in_z \sin(\omega t/2) \\ i(n_x + in_y) \sin(\omega t/2) \end{pmatrix}. \tag{2.16}$$

The reader should verify that $|\psi(t)\rangle$ is normalized at any instant of time $t > 0$.

If $|\psi\rangle$ is an eigenstate of $H$, $|\uparrow_Z\rangle$ or $|\downarrow_Z\rangle$, the only effect is a change in the global phase of the state which has no physical consequences:

$$|\psi(t)\rangle = e^{-iE_0 t/\hbar}|\uparrow_Z\rangle \text{ or } e^{+iE_0 t/\hbar}|\downarrow_Z\rangle$$

Because of this, we call these *stationary states*. Similarly, we could have a uniform field in the $X$ direction or the $Y$ direction. In these cases, the Hamiltonians would be $E_0X$ or $E_0Y$, and the stationary states would be the X or Y eigenstates.

If the Hamiltonian $H(t)$ is not constant, the situation is more complicated; but the time evolution in every case is still given by a unitary transformation.

# Controlling the Hamiltonian

A common situation in quantum information is when we have some control over the Hamiltonian of the system. For instance, we could turn on a uniform magnetic field in the $Z$ direction, leave it on for a time $\tau$, and then turn it off. In that case, the state will have evolved by

$$|\psi\rangle \to \exp(i\theta\hat{Z})|\psi\rangle \equiv \hat{U}|\psi\rangle,$$

where $\vartheta = -E_0\tau/hbar$. In this case, we say we have "performed a unitary transformation U on n the system." The Hamiltonian has the time dependence $H(t) = f(t)E_0Z$, where $f(t) = 1$ for $0 \leq t \leq \tau$ and $f(t) = 0$ otherwise.

# Postulate 3: Measurement

An observable is a measurable quantity, which is associated with an Hermitian operator $O = O^{\dagger}$. In measuring an observable O,the possible measurement outcomes are given by the eigenvalues $\lambda_j$; these occur with probabilities equal to the square of the amplitude for that outcome, and the system is left in an eigenstate of O.

Suppose one is given a system in a state $|\psi\rangle$, and wishes to make a measurement of an observable $\hat{O}$. By the spectral theorem

$$\hat{O} = \sum_{j=1}^{M} \lambda_j \hat{\mathcal{P}}_j, \quad \sum_{j=1}^{M} \hat{\mathcal{P}}_j = \hat{I}, \quad \hat{\mathcal{P}}_j \hat{\mathcal{P}}_k = \delta_{jk} \hat{\mathcal{P}}_j.$$

$M \leq D$ and the projectors $P_j$ are a decompostion of the identity.

The outcome $\lambda_j$ occurs with probability $p_j = \langle\psi| P_j |\psi\rangle$ $\langle P_j\rangle$, and the system is left in the (renormalized) state

$$|\psi'\rangle = \hat{\mathcal{P}}_j |\psi\rangle / \sqrt{p_j}.$$

This is called *Born's Rule*. The expectation value of the measurement outcomes is $\langle O\rangle = \langle\psi | O|\psi\rangle$.

If $M = D$, so the $P_j$ are projectors $|\varphi_j\rangle\langle\varphi_j|$ onto eigen- vectors of O, then we can write $|\psi\rangle$ in the eigenbasis:

$$|\psi\rangle = \sum \alpha_j |\phi_j\rangle.$$

Outcome $\lambda_j$ occurs with probability $p_j = |\alpha_j|^2$ and the system is afterwards left in the state $|\varphi_j\rangle$.

## Expectation values.

Given a state $|\psi\rangle$ and an opertor O, we can calculate a number

$$\langle\hat{O}\rangle \equiv \langle\psi|\hat{O}|\psi\rangle = \langle\psi|\left(\hat{O}|\psi\rangle\right)$$

which is called *the expectation value of Oin the state* $|\psi\rangle$. Given a particular choice of basis, we can express this number in terms of the elements of O and $|\psi\rangle$:

$$\langle\hat{O}\rangle = \sum_{i,j} \alpha_i^* a_{ij} \alpha_j$$

As we will see, when O is Hermitian, its expectation value gives the average result of some measurement on a system in the state $|\psi\rangle$.

# Postulate 4: Composite systems

If a composite system is composed of subsystems A and B which have associated Hilbert spaces $H_A$ and $H_B$, then the associated Hilbert space of the joint system is the tensor product space

$H_A \otimes H_B$.

Everything we have already learned about quantum mechanics generalizes to the case where the system is part of a composite system. Let's go through them point by point.

# Acting on a Subsystem

1. If subsystem A is in state $|\psi\rangle$ and subsystem B is in state $|\varphi\rangle$, then the *joint system* is in the product state $|\psi\rangle \otimes |\varphi\rangle$.

2. If $U_A$ is a unitary transformation which acts on subsystem A, then

$$U_A \otimes I$$

is the corresponding unitary for the joint system. Similarly, if $U_B$ acts on B, then $I \otimes U_B$ is the unitary for the joint system.

$$(\hat{U}_A \otimes \hat{I})(|\psi\rangle \otimes |\phi\rangle) = (\hat{U}_A|\psi\rangle) \otimes |\phi\rangle.$$

$$(\hat{I} \otimes \hat{U}_B)(|\psi\rangle \otimes |\phi\rangle) = |\psi\rangle \otimes (\hat{U}_B|\phi\rangle).$$

3. If A is an observable for subsystem A, then $A \otimes I$ is the corresponding observable for the joint system.

Note that $A \otimes I$ and $I \otimes B$ *always* commute, and therefore are compatible observables. Physically, this means that measurements on different subsystems can always be done simultaneously.

# Treating Subsystems Jointly

While we can extend the results for single systems to composite systems, there are many more possible states, evolutions and measurements that are allowed.

Most states $|\Psi\rangle$ of a composite system are *not* product states. For an example with two spin-1/2 systems,

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle$$

is not a product state. For this joint state, we cannot assign well-defined states to the subsystems. Such a joint state is called *entangled*.

A consequence of entanglement is that measurements on the subsystems will in general be *correlated*.

# Interactions

We can also perform joint unitaries U on both systems at once. If the initial state is a product $|\psi\rangle \otimes |\varphi\rangle$, then after applying a joint unitary the system will in general be entangled. Correlations are produced by *interaction* between the spins.

For example, we might have a Hamiltonian of the form

$$\hat{H} = E_0 \hat{Z} \otimes \hat{Z}.$$

The unitary operators $\exp(i\vartheta H)$ produced by this Hamiltonian will *not* be product operators, even though H itself *is* a product operator. So initial product states will evolve to become entangled.

# Joint Measurements

Finally, we can measure observables O which are *not* product operators. The measurement process follows the same rules we have already seen: an eigenvalue of O will occur with some probability, and the system will be left in the corresponding eigenstate of *O*. However, since O is not a product operator, the eigenstates of O will in general be *entangled* states.

This means that entanglement can be produced by joint measurements even if the initial state $|\psi\rangle \otimes |\varphi\rangle$ was a product.