5. Summary: Notation

Let us also at this point summarize some of the notation we have introduced and its corresponding meaning in the more familiar language of matrices and row vectors.

- A state is described by a ket or a bra, which in turn can be described as a column or row vector, respectively. The entries of these two vectors are then further related by complex conjugation.
- Observables are described by operators, which in turn are described by matrices. They act from the left on a ket and from the right on a bra:
$$A|\psi\rangle \leftrightarrow \langle\psi|A^\dagger, \tag{1.46}$$
where the Hermitian conjugate is denoted $A^\dagger$.
- The Hermitian conjugation acts on the matrix by complex conjugation together with transposition:
$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \implies A^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}. \tag{1.47}$$
- A normal operator is defined by $A^\dagger A = AA^\dagger$, or $[A^\dagger, A] = A^\dagger A - AA^\dagger = 0$, where $[\cdot,\cdot]$ is called the commutator.
- A Hermitian operator is defined by $A^\dagger = A$, it has real eigenvalues.
- A unitary operator is defined by $U^\dagger U = \mathbb{1}$.

6. What actually is the quantum state?

At this point, you might be asking yourself what the meaning of the quantum state is. After all, measurements tells us that eventually the state will not be in a superposition, the thing we observe is a definitive classical state, so how do we know that the state was ever in a superposition of other states? Well, such questions have given rise to a large number of debates on the interpretation of quantum mechanics. [14]

Many early interpretations of quantum mechanics involved hidden variables, i.e., that there are some hidden variables that we do not know about which determines the measurements in a deterministic fashion. These have been essentially refuted by a number of results, such as Gleason's theorem and variations thereof. These type of results typically go under the name of Bell's theorem, and in principle they rule out almost all hidden variables theories. The experimental verification of these results was the subject of the Nobel prize in physics 2022.[15]

In contrast, the widely considered Copenhagen interpretation of quantum mechanics (with variations) is essentially Bayesian. In this interpretation, the nature of quantum mechanics is essentially non-deterministic, and we should not require one to consider the "exponential" dimension of the quantum state prior to measurement any more so than we require a person throwing a die to consider the probability distribution over the outcomes. Measurements give rise to a (practically) irreversible process in which the state is affected.

Another famous interpretation is the many-worlds interpretation due to Hugh Everett. Here, time is considered as a tree, having many branches and each branch corresponds to a possible result of a measurement. This gives rise to an uncountable number of worlds or universes. The many-worlds interpretation is thus inherently deterministic, as the universal wave function never collapses to one particular state.

Finally, let us mention the de Broglie-Bohm interpretation. This is a kind of hidden variables theory where the problems of Bell's theorem are circumvented by embracing non-locality. Locality is basically the concept that only things near to each other can affect each other. This is one of the main building

[14] See for example Wikipedia

[15] Awarded to the three experimentalists Alain Aspect, John Clauser and Anton Zeilinger.

blocks of Einstein's theory of special relativity. The de Broglie-Bohm interpretation is thus a deterministic theory and particles have a definite configuration at all times, even when not observed. This has gained some interest in recent years and researcher are currently working on how to align it with the ideas of special relativity.

7. The harmonic oscillator

To give some intuition, as well as motivation, for the many concepts we have introduced we will now study the harmonic oscillator. This is a very important system in physics, if not the most important. A vast number of physical systems can be described using the harmonic oscillator. It also plays a big role in various physical implementations of qubits. We will begin with the classical harmonic oscillator and then study the quantum version, highlighting the differences.

7.1. The classical harmonic oscillator. Classical systems follow Newton's laws of mechanics. In particular, the second law states that the force is equal to the mass times the acceleration,

$$F = ma. \tag{1.48}$$

A harmonic oscillator is a particle that undergoes harmonic motion around an equilibrium point. Think for example of a spring with a mass attached to its end such that it bounces back and forth around an equilibrium.

Let us focus on the one-dimensional case and set the equilibrium point to be $x = 0$. The system is described by a mass m and a restoring force that pushes the mass towards the equilibrium point,

$$F = -m\omega^2 x, \tag{1.49}$$

where ω is called the angular frequency. The minus sign tells us that the force is driving the spring back towards its equilibrium point. Combining this with Newton's second law we get

$$ma = m\ddot{x} = -m\omega^2 x. \tag{1.50}$$

The solution of this second order differential equation is

$$x(t) = A\cos(\omega t + \phi), \tag{1.51}$$

where A is the amplitude of the oscillations (giving the turning points of the motion) and ϕ the initial phase.

The potential energy of the system is given by

$$V = \frac{1}{2}m\omega^2 x^2. \tag{1.52}$$

This gives a parabola as shown in Figure 1.1. The reason why the harmonic oscillator is so important is that almost any smooth function can be approximated by a parabola near its minimum points.

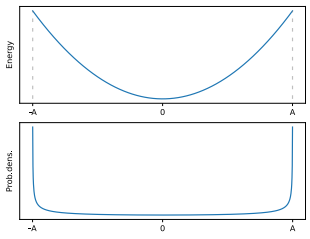

FIGURE 1.1. The potential energy (top) and probability density (bottom) of the classical harmonic oscillator, with amplitude A.

Remember that the total energy of the system is given by the sum of the potential energy, V, and the kinetic energy $\frac{1}{2}mv^2$. At the turning points $x = \pm A$, the velocity, and therefore the kinetic energy, is zero, and the potential energy reaches its maximum. The total energy of the system thus simply says something about how far away from the equilibrium it can move. For example, the zero-energy harmonic

oscillator simply sits still at its equilibrium. At the equilibrium point, on the other hand, the kinetic energy reaches its maximum and the potential energy is zero, this means that the particle attains the greatest velocity at this point. This further implies that for a classical harmonic oscillator, the probability is highest to find it close to the turning points $x = \pm A$, since this is where it moves at its slowest, and thus spends the most time. This is shown in the bottom picture of Fig. 1.1.

7.2. The quantum harmonic oscillator. The quantum harmonic oscillator is the quantum analogue of the classical system. As we discussed earlier, in quantum mechanics (and also in classical mechanics) an important role is played by the Hamiltonian of the system. This is simply constructed as the sum of the kinetic and potential energy. So to construct the quantum Hamiltonian we simply take the expression for the classical kinetic and potential energy and sum them. But in quantum mechanics, as we have seen, observables should be operators, so we also promote the position and momentum ($p = mv$) variables to operators.[16] This results in the expression

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \tag{1.53}$$

where we, in this section only, adopted the very common practice of putting hats on quantum operators, to distinguish them from their classical variable analogues. Note that, in contrast to the rest of this course, we are here considering an infinite-dimensional Hilbert space of states, since both $\hat{x}$ and $\hat{p}$ take continuous values. This does introduce some extra subtleties that we however simply gloss over at the moment.

In quantum mechanics, as we have seen earlier, the energy of the system is described by the time-independent Schrödinger equation

$$\hat{H}|\psi_E\rangle = E|\psi_E\rangle, \tag{1.54}$$

where the subscript E on ψ_E is there to remind us that these are the eigenvectors of $\hat{H}$ corresponding to the eigenvalues E. To solve this, we express the wave function $\psi_E(x) = \langle x|\psi_E\rangle$ in the coordinate basis. In this basis we can represent the momentum operator $\hat{p}$ as a derivative $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, and the equation takes the form

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E(x)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi_E(x) = E\psi_E(x). \tag{1.55}$$

This does not look like something we want to explicitly solve in this course, you can take a more advanced course on quantum mechanics or differential equations for that.[17] Here we simply state that under the assumptions that the wave function is normalizable and symmetric around the equilibrium $x = 0$, we have an infinite family of solutions labeled by a level (or *quantum number*) n

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad n = 0, 1, 2, \ldots. \tag{1.56}$$

Here, $H_n(y)$ are the so called (physicist's) Hermite polynomials, with the first few being

$$\begin{aligned} H_0(y) &= 1, \\ H_1(y) &= 2y, \\ H_2(y) &= 4y^2 - 2, \\ H_3(y) &= 8y^3 - 12y, \\ &\vdots \end{aligned} \tag{1.57}$$

The corresponding energy eigenvalues are

$$E_n = \hbar\omega(n + \tfrac{1}{2}). \tag{1.58}$$

These are the values that would be returned upon a measurement of the Hamiltonian of the quantum harmonic oscillator. Two important things to note are, first that the energies are quantized, i.e., they

[16] There are many reasons why we use momentum instead of velocity as the go-to operator in quantum mechanics, the most important one being that momentum is a conserved quantity, while velocity is not.

[17] Of course you are welcome to solve it yourselves. A nice trick one can use is to first guess or argue for the expression of the lowest energy state, and then use the fact that $[\hat{x}, \hat{p}] = i\hbar$ together with the algebra given by introducing the *creation* and *annihilation* operators $a^{\pm} \propto \hat{p} \pm i\omega\hat{x}$ to construct the higher energy states.

come in discrete steps; and secondly the lowest value is not equal to zero, but rather $E_0 = \frac{\hbar\omega}{2}$. This second point is a consequence of the famous Heisenberg's uncertainty principle, which in turn is a consequence of the fact that non-commuting observables are not simultaneously diagonalizable, as we mentioned before.

To connect with the classical system we can calculate the amplitudes, A_n, of a classical harmonic oscillator with the corresponding energies of the quantum one. We find

$$E_n = \frac{1}{2}m\omega^2 A_n^2 \implies A_n = \sqrt{(2n+1)\frac{\hbar}{m\omega}}. \tag{1.59}$$

Note that these increase with the quantum number n.

Figure 1.2 shows the probability amplitudes, $\psi_n(x)$, and probability densities, $|\psi_n(x)|^2$ of finding the system at the location x, for the first few energy levels in the positional basis. We note two big differences with the classical oscillator. First, there is a non-zero probability of finding the particle outside the values $x = \pm A_n$, this is not possible in the classical system. This is due to something called *quantum tunneling*. Secondly, the probability density distribution for the lowest-energy state $\psi_0(x)$, is highest at the origin $x = 0$, while for the higher values of n we see that the system starts looking more like the classical one, i.e., that it is most likely to find the system near the turning points. This is an illustration of something called the Bohr correspondence principle. Namely that quantum physics should become classical physics in the limit of large quantum numbers (or when $\hbar$ becomes small in comparison to the energy).

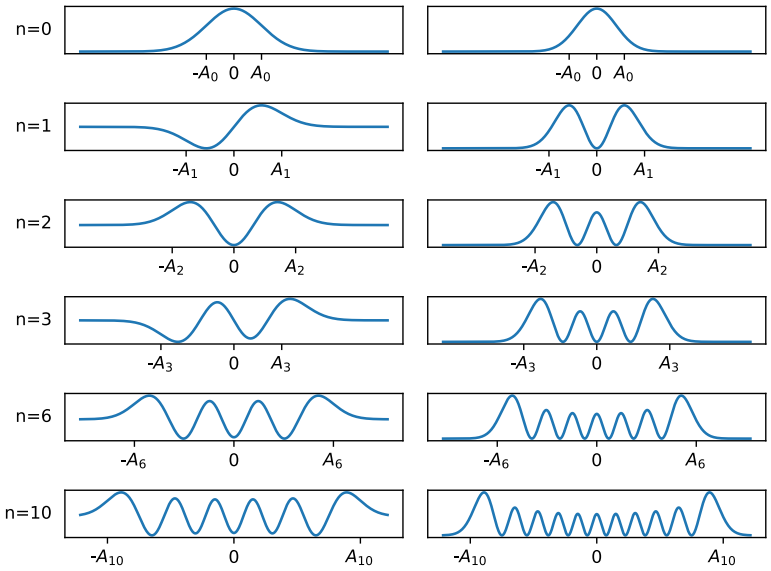

FIGURE 1.2. The probability amplitudes (left) and probability densities (right) for some levels of the quantum harmonic oscillator. The classical amplitudes A_n are indicated.

8. The qubit

Let us now introduce the main protagonist of the course, the qubit. In a classical computers we use bits that are systems whose states takes values 0 or 1. The corresponding quantum system is called a *qubit* (sometimes QBit, q-bit or quantum bit). This system is described by a two-dimensional complex vector space. To make the connection to classical bits even stronger we denote a set of basis vectors in this state space as

$$\{|0\rangle, |1\rangle\}. \tag{1.60}$$

Note that, as was mentioned before, we use here the notation $|0\rangle$ to denote a basis vector, not the zero element. This basis is typically referred to as the *computational basis*. Another frequently appearing basis is given by the states

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle). \tag{1.61}$$

You may recognize these bases as the u, d and l, r basis we studied earlier. The $|\pm\rangle$ basis is sometimes called the Hadamard basis. Any qubit can be expanded in either of these bases,

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle = \alpha_+|+\rangle + \alpha_-|-\rangle, \tag{1.62}$$

for some numbers α_j, with the extra condition $|\alpha_0|^2 + |\alpha_1|^2 = |\alpha_+|^2 + |\alpha_-|^2 = 1$.

We will often represent the computational basis by the vectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1.63}$$

Linear operators acting on a qubit will now be described by 2×2 complex matrices. Of special importance are the so called *Pauli operators*.[18] These are a set of three matrices that together with the identity matrix spans the vector space of 2×2 Hermitian matrices. In the computational basis, they read

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.64}$$

As an easy, but informative, exercise, we can study how the Pauli operators act on the basis states. This will be very helpful later when we want to start building quantum circuits. We find[19]

$$\sigma_x \begin{Bmatrix} |0\rangle \\ |1\rangle \\ |+\rangle \\ |-\rangle \end{Bmatrix} = \begin{Bmatrix} |1\rangle \\ |0\rangle \\ |+\rangle \\ -|-\rangle \end{Bmatrix}, \quad \sigma_y \begin{Bmatrix} |0\rangle \\ |1\rangle \\ |+\rangle \\ |-\rangle \end{Bmatrix} = \begin{Bmatrix} i|1\rangle \\ -i|0\rangle \\ -i|-\rangle \\ i|+\rangle \end{Bmatrix}, \quad \sigma_z \begin{Bmatrix} |0\rangle \\ |1\rangle \\ |+\rangle \\ |-\rangle \end{Bmatrix} = \begin{Bmatrix} |0\rangle \\ -|1\rangle \\ |-\rangle \\ |+\rangle \end{Bmatrix}. \tag{1.65}$$

When discussing quantum gates, the σ_x operator is sometimes referred to as the NOT gate, since it interchanges $|0\rangle$ and $|1\rangle$.

8.1. The Bloch sphere. We know that we can express any qubit as a superposition of the two basis vectors $|0\rangle$, $|1\rangle$, and that the corresponding coefficients must satisfy $|\alpha_0|^2 + |\alpha_1|^2 = 1$. We can then use a little trigonometry to express any qubit as

$$|\psi\rangle = e^{i\gamma}\left(\cos\tfrac{\theta}{2}|0\rangle + e^{i\phi}\sin\tfrac{\theta}{2}|1\rangle\right). \tag{1.66}$$

Where γ, ϕ and θ are some real numbers. However, we also saw earlier that that we can not distinguish states that only differ by an overall phase, so we can disregard the overall phase factor $e^{i\gamma}$. We can thus describe any qubit in terms of two real numbers ϕ and θ through the identification

$$|\psi\rangle = \cos\tfrac{\theta}{2}|0\rangle + e^{i\phi}\sin\tfrac{\theta}{2}|1\rangle. \tag{1.67}$$

This is simply the spherical coordinates for the unit sphere, and we have thus found that any qubit can be represented by a point on the unit sphere. This representation of the state space as a sphere goes under the name of the *Bloch sphere*.

Figure 1.3 shows how we can visualize the state $|+\rangle$ on the Bloch sphere.

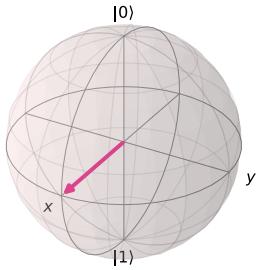

FIGURE 1.3. The Bloch sphere. The vector denotes the qubit state $|\psi\rangle = |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. The labels x and y represent the Euclidean x and y directions.

[18] Named after the Austrian physicist Wolfgang Pauli, who is counted as one of the main inventors of quantum mechanics.

[19] Perhaps you recognize some of these properties from when we studied the up/down/left/right system earlier.

It can be easily seen from the previous calculations that the Pauli matrices act as rotations along the different axes of the Bloch sphere. For example, acting with σ_x on $|0\rangle$ rotates the state 180°, or π radians, around the x-axis to give the state $|1\rangle$, and so on. All the standard one qubit gates can be visualized in a similar manner as their action on the sphere.

8.2. Several qubits. As we discussed previously, we can combine simple systems into larger ones by using the tensor product of vector spaces. This will be vital when constructing quantum circuits, since obviously, having just one qubit would perhaps not be all that exciting.

So, using the tensor product we can build larger systems of several qubits, for example

$$|0\rangle \otimes |0\rangle \otimes |+\rangle \otimes |1\rangle \otimes \cdots \otimes |1\rangle. \tag{1.68}$$

We will often be lazy and use the notation

$$|\psi_{n-1} \dots \psi_0\rangle \coloneqq |\psi_{n-1}\rangle \otimes |\psi_{n-2}\rangle \otimes \cdots \otimes |\psi_0\rangle. \tag{1.69}$$

For example, for the two-qubit system, given by a four-dimensional vector space, we then have the basis vectors

$$|00\rangle = |0\rangle \otimes |0\rangle, \quad |01\rangle = |0\rangle \otimes |1\rangle, \quad |10\rangle = |1\rangle \otimes |0\rangle, \quad |11\rangle = |1\rangle \otimes |1\rangle. \tag{1.70}$$

It is easy to show that these span the vector space of states. Sometimes a further simplification of notation is used for these types of combined systems where we imagine the product to indicate a binary representation of an integer, so that we write for example $|01\rangle = |1\rangle_2$ and $|11\rangle = |3\rangle_2$ and so on, where the subscript indicates how many qubits there are in the system. The subscript is of course needed because 001 and 1 are both binary representations of the number 1, while here the former would be a three qubit system and the later a one qubit system.

9. Building our first quantum circuits

We are now ready to start building quantum circuits. The ingredients will be qubits and unitary operators or gates.

First of all we need to discuss where we will start, i.e., what is the initial state of the system, or the input of the circuit, and how do we prepare that? A simple choice of input vector that is most commonly used is to pick $|0 \dots 0\rangle$ as the initial state vector. Given some general initial state, how do we prepare it in the $|0 \dots 0\rangle$? Well, one very simple way is found by remembering that measurements will make the system collapse to a given eigenvector of the observable being measured. We can then simply make a measurement of σ_z on each qubit, which will return the results ± 1 with some probabilities. If we get $+1$ we know that the qubit is in the state $|0\rangle$ as desired, while if we find -1 we know that it will be in the state $|1\rangle$. Then we simply keep the qubits that are in the $|0\rangle$ state and act with σ_x on the others, since we saw previously that $\sigma_x|1\rangle = |0\rangle$. Now we have our input vector $|\psi\rangle = |0 \dots 0\rangle$.

The quantum circuit will then start with a number of qubits in the $|0\rangle$ state and act on this with some number of gates, or unitary operators. The most basic gates are:

- The Pauli matrices: σ_x, σ_y and σ_z. These are typically denoted by X, Y and Z in the circuit diagrams. On the Bloch sphere we can visualize them as a π-rotation of the qubit about the corresponding axis.

- The Hadamard gate: $H \coloneqq \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$. It changes $|0\rangle \to |+\rangle$ and $|1\rangle \to |-\rangle$. So it can be seen as a change of basis. On the Bloch sphere we can visualize it as a π-rotation about the axis $\frac{1}{\sqrt{2}}(\hat{x} + \hat{z})$.

- Phase shift gates changes the relative phase in the expansion in the computational basis by sending $|0\rangle \to |0\rangle$ and $|1\rangle \to e^{i\varphi}|1\rangle$. Common examples are the T gate, with $\varphi = \pi/4$,[20] and the S gate, where $\varphi = \pi/2$. On the Bloch sphere, these gates can be seen as a rotation of φ radians about the $\hat{z}$ axis.

[20] the T gate is confusingly also known as the $\pi/8$ gate,

- The controlled-U gate acts on a number of qubits and uses the first as a control. If this is $|0\rangle$ it does nothing, while if it is $|1\rangle$ it acts on the second qubit with the operator U. For example, the controlled-X, or CNOT, gate, is a two qubit gate that acts in the following way:

$$\begin{aligned} |00\rangle &\to |00\rangle, \\ |01\rangle &\to |01\rangle, \\ |10\rangle &\to |1\rangle \otimes \sigma_x|0\rangle = |11\rangle, \\ |11\rangle &\to |1\rangle \otimes \sigma_x|1\rangle = |10\rangle. \end{aligned} \tag{1.71}$$

- The Toffoli, or CCNOT, gate is a controlled-controlled-gate acting on three qubits. If the two first qubits are in the state $|1\rangle$ then it acts on the third with the X gate. Otherwise it does nothing. We can thus represent it as the matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{1.72}$$

The Hadamard, CNOT and S gates together generate a group called the Clifford group. But it is important to note that, due to the Gottesman-Knill theorem, the Clifford gates does not make a universal gate set. However, the Hadamard together with the Tofolli gate is a universal set. Other combinations are also common as universal gate sets.

Two example circuits are given in Figures 1.4 and 1.5. One important thing to note is that when we read the circuits we read it from left to right, but when we write it down mathematically the gates act in the opposite order. In other words, the circuit of Fig. 1.4 would read

$$|0\rangle \otimes |+\rangle \otimes |-\rangle = |0\rangle \otimes \mathrm{H}|0\rangle \otimes \mathrm{H}\sigma_x|0\rangle. \tag{1.73}$$

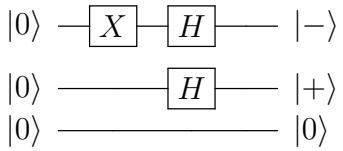

FIGURE 1.4. A simple example of a quantum circuit using the X and H gates.

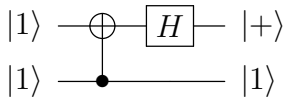

FIGURE 1.5. A simple example of a quantum circuit using the H and CNOT gate.

Finally, after we have acted with all of our gates in the circuit we want to retrieve the result. This is done by simply measuring the desired properties of the final state.

10. Physical implementations

There are several physical implementations of a qubit, including:

- Superconducting qubits: These qubits are made from tiny loops of superconducting wire, which can carry electrical current without resistance. The state of a superconducting qubit can be controlled by applying electromagnetic pulses to the loop.
- Trapped-ion qubits: These qubits are made by trapping a single ion (an electrically charged atom) in a magnetic or electric field. The state of a trapped-ion qubit can be controlled by shining laser light on the ion.
- Topological qubits: These qubits are based on the properties of certain materials, such as topological insulators, that can carry electrical current on their surface while insulating inside.
- Quantum dots: These qubits are made by confining a single electron or hole (an absence of an electron) in a tiny semiconductor structure called a quantum dot.
- Nuclear Magnetic Resonance (NMR) qubits: These qubits are based on the spin of the nuclei of certain atoms.
- Photonic qubits: These qubits are based on the properties of individual photons (particles of light). For example, the polarization state of a photon can be used as a qubit, with the two possible states being horizontal and vertical polarization.
- Single-molecule spin qubits: These qubits are based on the spin of individual electrons or nuclei in a single molecule. The state of the qubit can be controlled by applying magnetic fields to the molecule. These qubits are still in the research stage and not yet commercialized.