# Complex Inner product spaces and formulation of quantum theory

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"If you think you understand **quantum mechanics**, you don't understand **quantum mechanics**."

-Richard Feynman

**Introduction**

Classical physics is only an approximation of physics that works for large objects. To describe the behavior of the building blocks of nature, we need a radically different approach that leads to quantum mechanics. If we try to describe the behavior of atoms and their constituents like protons, neutrons and electrons using the laws of classical physics, it completely fails. For instance, if we described the motion of electrons around the nucleus of an atom using classical principles, we can calculate that any atom would collapse within a tiny fraction of a second[1]. Thus, quantum mechanics explains the phenomenon that classical physics cannot. Quantum mechanics refers to the description of the behavior of building blocks of nature like atoms, molecules, photons, etc.

Linear algebra is used widely in quantum mechanics. We will see how to use linear algebra to quantify and model these physical phenomena of quantum mechanics. For example, we say that the two wave functions are orthogonal to each other. It means that the waves can be represented as vectors that are have their inner product as 0.

There are five postulates that fully encapsulate the mathematical modelling of quantum mechanics. We divided these postulates across team members so that we could gain a deeper understanding of each postulate. I learnt about the first postulate and explained it to my team members. Fifth postulate was explained by Prudhvi and the Heisenberg's principle was explained by Revanth. I read the rest of the postulates from the references given at the end of the report.

**Pre-requisites** to understand Postulate 1: Inner product, Hilbert space definition, Orthogonal vectors, Basis

Inner product: Like the vector space has addition and scalar multiplication operators, the Hilbert space has an extra operator called the "inner product". It operates on two vectors and returns a scalar number. If the two vectors are $\vec{v}$and $\vec{w}$, then the inner product is denoted by:

$$\vec{v}.\ \vec{w}\ =\ \sum_{j=1}^{n} \bar{v_j} w_j$$

Here, $\bar{v_j}$ represents the conjugate of a complex number $v_j$.

$$\text{If } v_j = a + ib\,,\ then\, \bar{v_j} = a - ib.$$

**Vector representation of inner product**

$$\text{If } v = \begin{bmatrix} v_1 \\ v_2 \\ . \\ . \\ v_n \end{bmatrix} \text{ and } w = \begin{bmatrix} w_1 \\ w_2 \\ . \\ . \\ w_n \end{bmatrix} \text{ then}$$

$$\vec{v}.\ \vec{w}\ =\ \bar{v_1}w_1\ +\ \bar{v_2}w_2\ +\ldots+\bar{v_n}w_n$$

Example: If

$$\vec{v}=\begin{bmatrix} i \\ 2+i \end{bmatrix} and\, \vec{w}=\begin{bmatrix} 2 \\ -1 \end{bmatrix}$$

Then the inner product of these two vectors can be calculated as:

$$\vec{v}.\ \vec{w}\ =\ (-i).2\ +\ (2-i).(-1)$$

**Matrix representation of inner product**

We can also represent this using a matrix representation compactly. Taking the inner product of $\vec{v}$ and$\vec{w}$ is the same as doing a matrix multiplication between $\vec{v}^{\theta}$and $\vec{w}$.

Here, $\theta$ means first we take the complex conjugate of each element in the vector and then we take the transpose of that vector.

$$\vec{v}^{\theta}\cdot\vec{w}=\begin{bmatrix}\bar{v_1} & \bar{v_2} & \ldots & \bar{v_n}\end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

$$=\bar{v_1}w_1\ +\ \bar{v_2}w_2\ +\ldots+\bar{v_n}w_n$$

$$=\vec{v}\cdot\vec{w}$$

So,

$$\vec{v}\cdot\vec{w}=\vec{v}^{\theta}\cdot\vec{w}$$

Inner products allow the rigorous introduction of intuitive geometrical notions, such as the length of a vector or the angle between two vectors. They also provide a means of defining orthogonality between vectors (zero inner product).

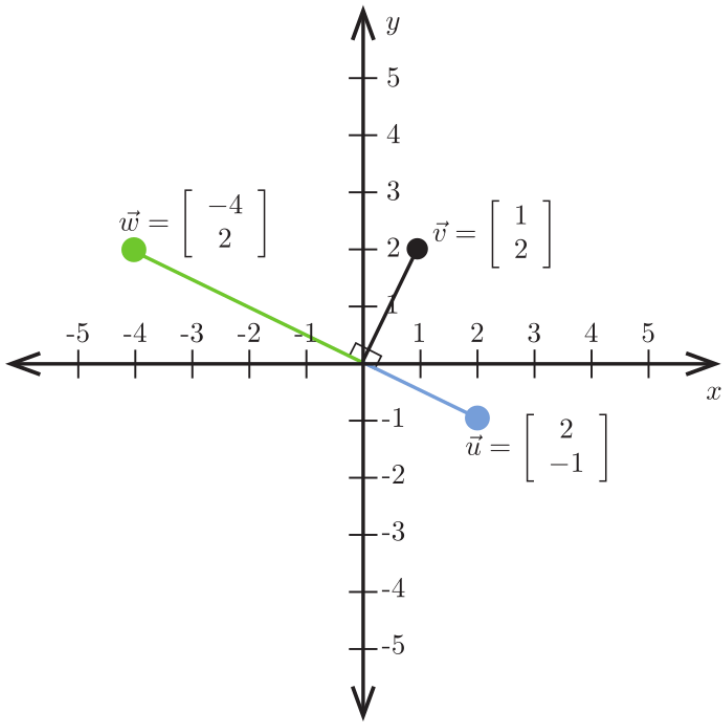
**Orthogonal vectors**

Orthogonal vectors are vectors that have an angle of 90° between them. We say that two vectors are orthogonal, or perpendicular, if their inner product is 0.

For example, let us consider three vectors:

$$\vec{v}=\begin{bmatrix}1\\2\end{bmatrix},\ \vec{w}=\begin{bmatrix}-4\\2\end{bmatrix}\text{ and }\vec{u}=\begin{bmatrix}2\\-1\end{bmatrix}$$

The dimensions of all the vectors are 2. So, let us look at their representation in the 2D cartesian plane.




Through this visual representation, we see that $\vec{v}$ is perpendicular to both, $\vec{w}$ and $\vec{u}$. So, let us check if the inner product gives us the same result or not from a mathematical approach.

$$\begin{aligned}\vec{v} \cdot \vec{w} &= \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} -4 \\ 2 \end{bmatrix} \\ &= (-1).4 + 2.2 \\ &= 0\end{aligned}$$

Also,

$$\begin{aligned}\vec{v} \cdot \vec{u} &= \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 2 \\ -1 \end{bmatrix} \\ &= 1.2 + 2.(-1) \\ &= 0\end{aligned}$$

So, we can see that the inner product does give us the result as 0 for two orthogonal vectors.

**Hilbert Space**

A vector space with a well-defined inner product is called a Hilbert space. The collection of all the n-dimensional vectors with the inner product as defined above form a Hilbert space.

Definition of Hilbert Space [2]:

a) It is a vector space over the complex numbers C. Vectors will be denoted as $|\psi\rangle$ (Dirac's ket-notation).

b) It has an inner product $\langle\psi|\phi\rangle$ that maps an ordered pair of vectors to C, and that has the properties:

I) Positivity: $\langle\psi|\psi\rangle > 0$ for $|\psi\rangle \neq 0$

II) Linearity: $\langle\phi|(a|\psi 1\rangle + b|\psi 2\rangle) = a\langle\phi|\psi 1\rangle + b\langle\phi|\psi 2\rangle$

III)Skew symmetry: $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^{*}$.

(The $*$ denotes complex conjugation.)

c) It is complete in the norm $||\psi|| = \langle\psi|\psi\rangle^{1/2}$.

(Completeness is an important proviso in infinite-dimensional function spaces since it ensures the convergence of certain eigenfunction expansions. But mostly we will be content to work with finite-dimensional inner-product spaces.)

Ray is an equivalence class of vectors that differ by multiplication by a nonzero complex scalar. For any nonzero ray, we can by convention choose a representative of the class, denoted by $|\psi\rangle$ , that has unit norm: $\langle\psi|\psi\rangle = 1$.

**Basis**

A basis is a finite set of vectors that can be used to describe any other vectors of the same dimension. Any set of n linearly independent vectors in $C^n$ (or $R^n$ ) is called a basis of $C^n$ (or $R^n$).

We say a basis is orthonormal if each vector has norm 1 and each pair of vectors are orthogonal.

**POSTULATE 1:**

A state is a complete description of a physical system. In quantum mechanics, a state is a ray in a Hilbert space.

Here, the quantum state refers to the collection of all relevant physical properties of a quantum system (e.g., position, momentum, spin, polarization).

**Exclusive and non-exclusive states**

Exclusive states: When modelling the state of a given physical quantity (position, spin, polarization), two states are said to be exclusive if the fact of being in one of the states with certainty implies that there are no chances of being in any of the other states.

Example 1: If there is a quantum particle and three quantum boxes and if we know that the particle is in the first box, then we can say for sure that it is not present in the second and third boxes. This system is said to have exclusive states.

Example 2: On the other hand, if we define three states as a particle moving horizontally, vertically or diagonally. A particle that moves diagonally can be thought to be moving simultaneously in horizontal and vertical directions. So, these three states are not mutually exclusive.

In linear algebra, we know that a vector does not have any common components with its orthogonal vector. Interestingly, the exclusivity of quantum states can be represented by orthogonal vectors. Given a quantum system with n-exclusive states, each state will be represented by a vector from an orthonormal basis of a n-dimensional Hilbert space.

In Example 1 stated above, the state of the electron can be in either box 1, 2, and 3 represented by the quantum state |1⟩, |2⟩ and |3⟩ respectively. Explicitly, we can write:

$$|1\rangle = \begin{bmatrix}1\\0\\0\end{bmatrix}, |2\rangle = \begin{bmatrix}0\\1\\0\end{bmatrix} and\ |3\rangle = \begin{bmatrix}0\\0\\1\end{bmatrix}$$

We can see that these vectors are orthogonal to each other (Linear Algebra Way). Another way of seeing it is the states represented by these vectors are exclusive (Quantum Mechanics Way)

We can also see that a state in quantum mechanics can be represented by a vector in Linear Algebra.

Another interesting concept is that of a **qubit**. In quantum information, we use quantum bits, or qubits. Like the classical bit, a qubit only has two exclusive states, “quantum-0” and “quantum-1”. But unlike the classical bit, the qubit behaves according to the laws of quantum mechanics. Just like the bit is the basic unit of classical information, the qubit is the basic unit of quantum information.

Since a qubit only has two different exclusive states, the state/vector representing the quantum-0 and the quantum-1 should be 2-dimensional. The vectors |0⟩ and |1⟩ are conventionally represented by the vectors:

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix} and |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$

We call this basis a computational basis.

**Example: Polarization of a photon as a qubit.**

If we use the energy of an electron in an atom as our quantum bit, we could say that the ground state (lowest energy) is our quantum-0, and an excited state (higher energy) is our quantum-1. Since the ground and excited states are mutually exclusive, we could represent:

$$ground\ state \leftrightarrow |0\rangle = \begin{bmatrix}1\\0\end{bmatrix} and\ excited\ state \leftrightarrow |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$

**Quantum superposition principle**

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

This can be written as

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

The above tells us that the states |±⟩ are linear combinations of the computational basis (i.e., the quantum-0 and quantum-1) It is possible for a system to be both state-0 and state-1.

If a quantum system can be in the state |0⟩, and can also be in |1⟩, then quantum mechanics allows

the system to be in any arbitrary state:

$$|\Psi\rangle = a|0\rangle + b|1\rangle = \begin{bmatrix}a\\b\end{bmatrix}$$

We say that |ψ⟩ is in a superposition of |0⟩ and |1⟩ with probability amplitudes a and b. The reason for such a name is that they do not represent a probability, but their modulus squared does give us the probability.

**POSTULATE 2:**

The probability of measuring a system in a given state is given by the modulus squared of the inner product of the output state and the current state of the system (Born's rule). Immediately after the measurement, the wavefunction collapses into that state.

Born's rule: Born's Rule. Suppose we have a quantum state |ψi and an orthonormal basis {|ϕ1⟩, . . . , |ϕn⟩}. Then we can measure |ψ⟩ with respect to this orthonormal basis, i.e., we "ask" the quantum system which one of these states it's in. The probability of measuring the state |ϕi⟩, P(ϕi), is given by:

$$P(\varphi_i) = |\langle \varphi_i | \psi \rangle|^2$$

Wave collapse: After the measurement is performed the original state collapses in the measured state, i.e., we're left with one of the states |ϕ1⟩, . . ., |ϕn⟩.

Quantum measurement: From a mathematical point of view, applying Born's rule and then the wave collapse corresponds to a quantum measurement.

Let us take an example to understand this. If we treat the general case of a qubit in an unknown quantum state |ψ⟩ = a|0⟩ + b|1⟩ and we measure in the computational basis, the outcome will be:

$$|0\rangle \; with \, \text{probability} \; |\langle 0|\Psi\rangle|^2 \; = \; |a|^2$$

$$|1\rangle \; with \, \text{probability} \; |\langle 1|\Psi\rangle|^2 \; = \; |b|^2$$

Now,

$$\langle \pm \, | \, w \rangle \; = \; \tfrac{1}{\sqrt{2}} [1 \quad \pm 1] \begin{bmatrix} a \\ b \end{bmatrix}$$

$$= \tfrac{a \pm b}{\sqrt{2}}$$

This implies that the outcome will be the state:

$$|\pm\rangle \; with \, \text{probability} \; \frac{|a \pm b|^2}{2}$$

Probabilism: Measuring in two different bases yields probabilistic measure. What the superposition principle and Born's rule are actually telling us is that quantum mechanics is inherently random. When we have an unknown quantum superposition, it's impossible to predict precisely which outcome we'll measure. We can only predict the probability of the outcome.

What this means is that if we are given a quantum state, we can calculate the probability with which it lies in any of the state.

**POSTULATE 3**

Quantum operations are represented by unitary operators on the Hilbert space.

Hadamard matrix(H) is a useful quantum operation.

$$H = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

When we perform a Hadamard operation on some matrices, we get the results that will lead us to an interesting phenomenon in quantum mechanics.

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = |+\rangle$$

$$H|1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = |-\rangle$$

$$H|+\rangle = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle$$

$$H|-\rangle = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} = |1\rangle$$

We can see that:

$$\begin{aligned} H|+\rangle &= \frac{1}{\sqrt{2}} H(|0\rangle + |\rangle) \\ &= \frac{1}{\sqrt{2}} (H|0\rangle + H|1\rangle) \\ &= \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle) \\ &= \frac{1}{2} (|0\rangle + |1\rangle + |0\rangle - |1\rangle) \\ &= |0\rangle \end{aligned}$$

The signs in front on both |0⟩ are the same, while the signs in front of both |1⟩ are opposite. This is an example of quantum interference. |0⟩ undergoes constructive interference and |1⟩ undergoes destructive interference. Interference is a property of waves and what you just saw is an example of the wave-particle duality inherent to quantum mechanics. This is an example of quantum interference. |0⟩ undergoes constructive interference and |1⟩ undergoes destructive interference. Interference is a

property of waves and what you just saw is an example of the wave-particle duality inherent to quantum mechanics.

Quantum operations are performed in various ways, depending on the quantum system we're trying to manipulate. If our qubit is represented by the polarization of a photon, we use quarter and half wave plates (essentially a piece of glass). If we use the ground and excited states of an atom, we can use a laser pulse. There are many different types of qubits and many ways to perform operations.

**POSTULATE 4:**

The Hilbert space of a composite system is given by the tensor product (also known as the Kronecker product) of the separate, individual Hilbert spaces.

**POSTULATE 5:**

This postulate was explained by Prudhvi.

Physical observables are represented by the eigenvalues of a Hermitian operator on the Hilbert space. For a given physically meaningful quantity with multiple possible values, there is a Hermitian operator that is associated with the possible value of the measurements.

The observable is physical quantity that can be measured. For example, energy, momentum, spin, etc. can be regarded as observables.

**Hermitian operator**

An operator Is a tool that extract useful information from quantum state, for example:

$$\hat{\hat{A}}f(x) = k * f(x)$$

Hermitian Operator is an operator whose conjugate transpose is equal to itself.

$M^{\dagger} = M$

The Eigen values of the Hermitian Operator are always real.

**Quantum mechanical theory**

The information about quantum system is contained within a mathematical entity called the wavefunction(ψ). Each physical property, or observable, of interest, has a corresponding operator which operates on the wavefunction. If the wavefunction is an eigenfunction of that operator, then its eigenvalue is the value of that observable.

A prime example of this is the Schrödinger equation:

$$\hat{H}\psi = E\psi$$

$$\left(\frac{h^2}{2m}\right) * \left(\frac{d^2\psi(x)}{dx^2}\right) + V(x) * \psi(x) = E\psi(x)$$

$$E_n = \frac{n^2 * h^2}{8mL^2}$$

Here by operating the Hermitian operator on the wave function, we get Energy as eigen value which is an observable of the particle.

Now that we have seen in detail about the five postulates of quantum mechanics, let us see how linear algebra relates to Heisenberg's uncertainty principle.

**Heisenberg's uncertainty principle**

This part was explained by Revanth.

The uncertainty principle says that we cannot measure the position(x) and the momentum(p) of a particle with absolute precision. The more accurately we know one of these values, the less accurately we know the other [3].

All physical observables must be represented by matrices. The set of eigenvalues of the matrix representing an observable is the set of all values that could arise as outcomes of experiments conducted on a system to measure the observable. Since the outcome of an experiment to measure a real observable must be a real number, Hermitian matrices would represent such observables (as their eigenvalues are real). If the result of a measurement is a certain eigenvalue, the corresponding eigenvector represents the state of the system immediately after the measurement. The act of measurement is taken to 'collapse' the state of the system to that eigenvector (or eigenstate). Examples of such eigenstates are those of position, momentum, energy, etc. It may be possible sometimes to make simultaneous measurements of two or more observables. In that case the system will collapse to a common eigen-state of these observables right after the measurement [4].

Further, from matrix theory we know that eigenvectors corresponding to distinct eigenvalues of a Hermitian matrix are orthogonal to each other. In this sense, they are analogous to the x y z axes of the Cartesian coordinate system -except that now there could even be an in-finite number of distinct eigen values, and hence as many mutually orthogonal eigenvectors 'pointing' along different independent directions in the linear vector space. Again, just as we have unit vectors $\hat{x}\,\hat{y}\,\hat{z}$ along the Cartesian axes, we can normalize each eigenvector to have unit magnitude. From $\hat{x}\,\text{and}\,\hat{y}$ , we can form a linear combination as:

$$f = a\hat{x} + b\hat{y}$$

where a and b are any two real numbers. In much the same way, linear superpositions of the normalized independent eigenvectors can be formed, with coefficients that are complex numbers. It is important to note that, in general, such superpositions are not the eigen states of the matrix concerned.

While a bit more nuanced, in quantum mechanics, a similar thing goes on with position and momentum. If we measure the position repeatedly, we will get the same answer each time. However, if we measure the momentum, the state will collapse to an eigenstate of the momentum operator, and, if we measured the position again, it would not be in the exact place anymore. In fact, if you measured the momentum perfectly, it turns out that you lose all position information. This underlies Heisenberg's uncertainty principle between position and momentum, which says that the product of the uncertainties for position and momentum $\sigma_x\sigma_y$must be at least a nonzero constant $\frac{\hbar}{2}$.

## CONCLUSION

We have understood how linear algebra can be used to model the phenomenon of quantum mechanics. We have discussed the five postulates of quantum mechanics in detail along with their applications. We then understood the relevance of Heisenberg's uncertainty principle.

## REFERENCES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[4] https://www.ias.ac.in/article/fulltext/reso/009/08/0046-0056