Lecture 2: Postulates Of Quantum Mechanics

from “quantum mechanics” by Claude Cohen-Tannoudji

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Postulates of Quantum Mechanics

- Postulates serve as hypotheses in Quantum Mechanics, forming the basis for making theoretical predictions within a mathematical framework. By comparing the outcomes of these predictions with experimental results, we validate and refine the postulates.

- Quantum Mechanics relies on a set of postulates, which are foundational hypotheses. These Postulates will provide us with an answer to the following questions:

(*i*) How is the state of a quantum system at a given time described mathematically?

(*ii*) Given this state, how can we predict the results of the measurement of various physical quantities?

(*iii*) How can the state of the system at an arbitrary time t be found when the state at time t_0 is known?

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Postulates of Quantum Mechanics

First Postulate: At a fixed time t_0, the state of a physical system is defined by specifying a ket $|\psi(t_0)\rangle$ belonging to the state space $\mathscr{E}$.

Classical Mechanics describes the dynamical* state variables of a particle as x, y, z, p, etc...

• Ψ(x, y ,z ,t) replaces the dynamical variables used in classical mechanics and fully describes a quantum mechanical particle.

Superposition: The wave function allows for superposition, meaning a quantum system can exist simultaneously in a combination of multiple states.

Probability: The absolute square of the wave function, |ψ|^2, gives the probability density of finding the system in a particular state or having specific measurement outcomes.

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Wave function: $\Psi(x, y, z, t)$

$\Psi(x, y, z, t)$ Should be single-valued, finite and continuous.

$\Psi(x,y,z,t)$, the particle "wave function", is related to the probability of finding a particle at time t in a volume dxdydz. Specifically, this probability is:

$$\left|\Psi(x,y,z,t)\right|^2 dxdydz \text{ or } \left[\Psi^*\Psi dxdydz\right]$$

But since Ψ is a probability,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|\Psi(x,y,z,t)\right|^2 dxdydz = 1$$

$$\text{or in 1D } \int_{-\infty}^{\infty}\left[\Psi^*\Psi dx\right] = 1$$

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Postulates of Quantum Mechanics

Second Postulate: Every measurable physical quantity $\mathscr{A}$ is described by an operator A acting in $\mathscr{E}$; this operator is an observable.

Where A is a Hermitian Operator. Properties of Hermitian Operator:

- Self-adjoint : $H^\dagger = H$
- Real eigenvalues
- Orthogonal Eigenvectors
- Probability Conservation

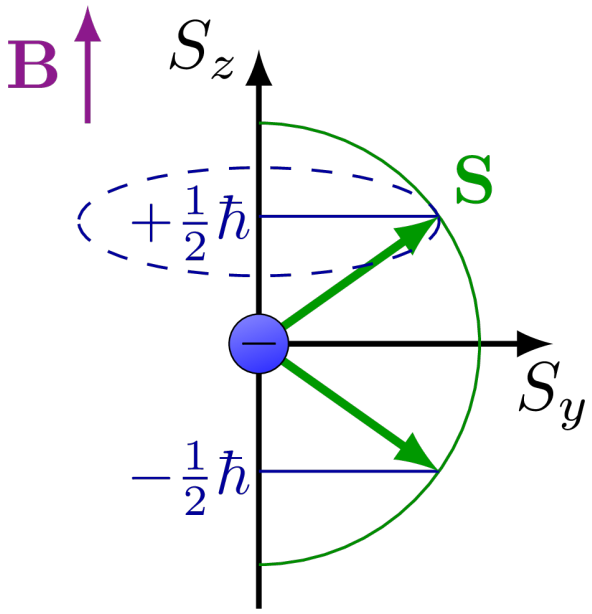
Classical Dynamical Variable	QM Operator Representation
Position x	x
Potential Energy V(x)	$V(x)$
f(x)	$f(x)$
Momentum p_x	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
Kinetic Energy $\frac{p_x^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
$f(p_x)$	$f\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$
Total Energy (Kinetic + Potential) E_{Total}	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
Total Energy (Time Version) E_{Total}	$-\frac{\hbar}{i}\frac{\partial}{\partial t}$

Postulates of Quantum Mechanics

Third Postulate: The only possible result of the measurement of a physical quantity $\mathscr{A}$ is one of the eigenvalues of the corresponding observable A.

$$S_z \chi_{s,m_s} = m_s \hbar \chi_{s,m_s},$$
$$S^2 \chi_{s,m_s} = s(s+1)\hbar^2 \chi_{s,m_s}.$$

- **S= 1/2 for fermions**
- **m_s= -1/2 or 1/2**



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Postulates of Quantum Mechanics

Fourth Postulate (case of a discrete non-degenerate spectrum): When the physical quantity $\mathscr{A}$ is measured on a system in the *normalized* state $|\psi\rangle$, the probability $\mathscr{P}(a_n)$ of obtaining the *non-degenerate* eigenvalue a_n of the corresponding observable A is:

$$\mathscr{P}(a_n) = |\langle u_n | \psi \rangle|^2$$

where $|u_n\rangle$ is the normalized eigenvector of A associated with the eigenvalue a_n.

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Postulates of Quantum Mechanics

Fifth Postulate: If the measurement of the physical quantity $\mathscr{A}$ on the system in the state $|\psi\rangle$ gives the result a_n, the state of the system immediately after the measurement is the normalized projection, $\frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}}$, of $|\psi\rangle$ onto the eigensubspace associated with a_n.

This postulate emphasizes that the act of measurement in quantum mechanics affects the state of the system, causing it to collapse into one of the possible eigenstates associated with the measured quantity.

After the measurement, the state of the system is always an eigenvector of the observable A with the eigenvalue an. It's important to note that the resulting state is not an arbitrary ket from the subspace Sn, but specifically the part of the original state $|\psi\rangle$ that belongs to Sn, appropriately normalized for convenience.

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Postulates of Quantum Mechanics

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

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

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

H is called the *Hamiltonian operator* of the system, as it is obtained from the classical Hamiltonian (appendix III and §5 below).

By solving the Schrödinger equation, we can determine how the state vector $|\psi(t)\rangle$ evolves in time, providing insights into the behaviour and properties of the quantum system.

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Physical Interpretation of Postulates Concerning Observables

1. The quantization rules in quantum mechanics are consistent with the probabilistic interpretation of the wave function. In the case of position and momentum observables, experiments show that all real values are possible for these variables. By applying the fourth postulate to these observables enables us to re-drive the probabilistic interpretation of wavefunctions.

Position Probability:

- For a one-dimensional scenario, the probability of measuring a particle's position between x and x + dx is given by : $d\mathcal{P}(x) = |\langle x | \psi \rangle|^2 \, dx$

- The square modulus, $|\langle x | \psi \rangle|^2$ represents the particle's position probability density.

Momentum Probability:

- Eigenvectors of the momentum observable correspond to plane waves with well-defined momentum.

- The probability of finding a particle in a state $|\psi\rangle$ with a momentum between p and p + dp is given by:

$$d\mathcal{P}(p) = |\langle p | \psi \rangle|^2 \, dp$$

the square modulus($|\langle p | \psi \rangle|^2$)of the wave function in momentum space.

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Physical Interpretation of Postulates Concerning Observables

2. Quantization of Certain Physical Quantities:

- The third postulate explains the quantization observed for certain quantities like the energy of atoms. Not all quantities are quantized, as some observables have a continuous spectrum.
- Predictions based on the third postulate have been successful in explaining and predicting experimental results, such as the quantization of energy levels in the hydrogen atom. They can also predict the energy values, which can be measured experimentally.

3. The Measurement Process:

- The fourth and fifth postulates raise fundamental questions about the measurement process in quantum mechanics. The particular question is of perturbation which arises when we consider measurement devices and systems independently.
- The nondeterministic nature of the postulates is related to the uncertainties and perturbations introduced during the measurement process. That's why we should only consider that the measurement devices used are perfect: that means assuming perturbation is only due to the quantum mechanical aspect of measurement.



Physical Interpretation of Postulates Concerning Observables

4. Mean Value of Observable in Given State:

The mean value of the observable** A in the state $|\psi\rangle$, which we shall denote by $\langle A \rangle_\psi$, or, more simply, by $\langle A \rangle$, is defined as the average of the results obtained when a large number N of measurements of this observable are performed on systems which are all in the state $|\psi\rangle$. When $|\psi\rangle$ is given, the probabilities of finding all the possible results are known. The mean value $\langle A \rangle_\psi$ can therefore be predicted. We shall show that if $|\psi\rangle$ is normalized, $\langle A \rangle_\psi$ is given by the formula :

$$\boxed{\langle A \rangle_\psi = \langle \psi | A | \psi \rangle} \qquad \text{(C-4)}$$

Case I: Mean Value Calculation: Discrete Spectrum

For discrete spectra, the mean value is the sum of eigenvalues weighted by their probabilities.

$$\langle A \rangle_\psi = \sum_n a_n \mathcal{P}(a_n)$$

Case 2: Mean Value Calculation: Continuous Spectrum

For continuous spectra, the mean value is the integral of results weighted by their probabilities.

$$\langle A \rangle_\psi = \int \alpha \, d\mathcal{P}(\alpha)$$

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Physical Interpretation of Postulates Concerning Observables

5. The root-mean-square deviation:

- The mean value < A > provides information about the average measurement result of an observable A in a given state.
- However, it doesn't capture the dispersion or spread of measurement results around < A >.We need a measure that characterizes the dispersion of measurement results.

By definition, we therefore introduce the *root-mean-square deviation* ΔA by setting:

$$\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} \qquad \text{(C-23)}$$

It can also be written as: $\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$

Connection to Heisenberg Uncertainty Principle

•Applying the root-mean-square deviation to observables R and P, we find an interesting connection to the Heisenberg uncertainty principle.

•For any state we have $\Delta R \cdot \Delta P \geq \hbar/2$, where ΔR and ΔP represent the uncertainties or root-mean-square deviations of R and P.

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Physical Interpretation of Postulates Concerning Observables

6. Compatibility of Observables:

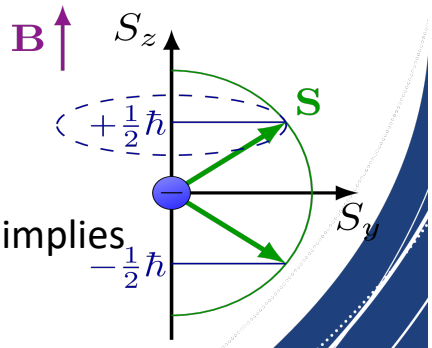
In quantum mechanics, observables are quantities that can be measured, such as position, momentum, energy, etc. The compatibility of observables refers to whether they can be simultaneously determined with certainty.

- The Commutator of two operators A, B is the operator C = [A, B] such that C = AB − BA.

Case I: If two observables, A and B, commute, it means that their commutator [A, B] is equal to zero. In this case, there exists a basis of the state space composed of eigenkets that are common to both observables.

Example: S and S_z commute i.e. $[S,S_Z] = 0$;

Case II: In this case, S_Z and S_X do not commute, which means they are incompatible. This implies that there is no common basis of eigenkets for Sz and Sx.



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The Physical Implications Of the Schrodinger Equation

- The Schrödinger equation describes the time evolution of a quantum system.

General properties of the Schrodinger equation :

1. Determinism in the evolution of the Physical system:

The Schrödinger equation:

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

If we have an initial state represented by the state vector $|\psi(t0)\rangle$, we can use the Schrödinger equation to calculate the state vector $|\psi(t)\rangle$ at any later time t.

2. The Superposition Principle:

The Schrödinger equation is linear and homogeneous, which means its solutions are linearly superposable. This principle allows us to combine multiple solutions of the equation to obtain new solutions.

Example: if $|\psi1(t)\rangle$ and $|\psi2(t)\rangle$ are solutions, then any linear combination of them, such as $A|\psi1(t)\rangle + B|\psi2(t)\rangle$ is also a valid solution.

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The Physical Implications Of the Schrodinger Equation

3. Conservation of Probability:

a. The Norm of the State Vector Remains Constant: The norm of the state vector, represented by $\langle\psi(t)|\psi(t)\rangle$, remains constant over time. This means that the total probability of finding the system in any state remains the same throughout its evolution.

Example: if we interpret the squared modulus of the wave function, |ψ(r, t)|^2, as the probability density of finding a particle at a particular position, the conservation of norm ensures that the total probability of finding the particle in all space remains equal to 1.

b. Local Conservation of Probability: The probability density, represented by |ψ(r, t)|^2, may vary with time at each point in space. This is similar to how charge density can vary in electromagnetism. However, the total probability within a given volume remains constant over time.

To describe the local conservation of probability, a probability current density, represented by J(r, t), is introduced.

$$\frac{\partial}{\partial t}\rho(\mathbf{r}, t) + \frac{\hbar}{2mi}\left[\psi^*(\mathbf{r}, t)\,\Delta\psi(\mathbf{r}, t) - \psi(\mathbf{r}, t)\,\Delta\psi^*(\mathbf{r}, t)\right] = 0$$

If we set :

$$\mathbf{J}(\mathbf{r}, t) = \frac{\hbar}{2mi}\left[\psi^*\nabla\psi - \psi\,\nabla\psi^*\right]$$

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The Physical Implications Of the Schrodinger Equation

4. Evolution of the Mean Value of an Observable: Relationship with classical Mechanics

The mean value of an observable A at a given time t is denoted as <A>(t). It is given by:

$$\langle A \rangle(t) = \langle \psi(t) | A | \psi(t) \rangle$$

The time evolution of the mean value of an observable follows from the Schrödinger equation. The observable A itself may also have an explicit dependence on time, which can cause an additional variation of <A>(t) with respect to time.

It's important to note that in quantum mechanics, the mean value of an observable is compared with the corresponding classical quantity at a specific time, not with the time-dependent classical quantity itself.

Example: In classical mechanics, the position and momentum of the oscillator explicitly depend on time and follow sinusoidal oscillations. However, in quantum mechanics, the position and momentum operators (observables) do not explicitly depend on time.



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The Superposition Principle and Physical Predictions

The superposition principle in quantum mechanics allows for the linear combination of states, and the resulting probabilities and outcomes of measurements depend on the complex probability amplitudes. This is distinct from a statistical mixture of states, and interference effects arise from the superposition, leading to unique physical predictions and phenomena in quantum mechanics.

- Example: Consider a photon in a state represented by the unit vector e = (ex + ey)/√2, which corresponds to linear polarization at an angle of 45° with respect to the ex and ey directions.
- If we consider a statistical mixture, we might assume that this state is equivalent to having N photons in the ex-polarization state and N photons in the ey polarization state. However, this is incorrect.
- As, if we place an analyzer with its axis perpendicular to e, none of the photons in the state e will pass through the analyzer. But if we had a statistical mixture with equal proportions of photons in the ex and ey states (representing unpolarized light), half of the photons would pass through the analyzer.

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We have Successfully Discussed:

- Postulates of Quantum Mechanics
- Physical Interpretation of Postulates Concerning Observables
- The Physical Implications Of the Schrodinger Equation
- The Superposition Principle and Physical Predictions