

A- Postulation of quantum theory

Postulate 1. The state of a quantum mechanical system is completely specified by a function $\psi (r; t)$ that depends on the coordinates of the particle(s) and on time. This function, called the wave function or state function, has the important property that $\psi^* (r; t) \psi (r; t) d\tau$ is the probability that the particle lies in the volume element $d\tau$ located at r at time t .

The wave function must satisfy certain mathematical conditions because of this probabilistic interpretation. For the case of a single particle, the probability of finding it somewhere is 1, so that we have the normalization condition

$$\int_{-\infty}^{\infty} \psi^*(r,t)\psi(r,t)d\tau = 1$$

It is customary to also normalize many-particle wave functions to 1². The wave function must also be single-valued, continuous, and finite.

Postulate 2. To every observable in classical mechanics there corresponds a linear, Hermitian operator in quantum mechanics. In this case if you like to write any physical quantity in quantum, first described it by classical physics and then changed into quantum mechanics

For example the kinetic energy, classically

$$K.E_x = \frac{1}{2} m u^2 \quad (38)$$

$$K.E_x = \frac{m^2 u^2}{2m} = \frac{P_x^2}{2m} \quad (39)$$

But momentum in quantum is

$$P_x = -\frac{i h}{2\pi} \frac{d}{dx} \quad (40)$$

Then substituted the value of momentum from eqn.39 in eqn 40 we get

$$K.E = \frac{1}{2m} \left(-\frac{i h}{2\pi} \frac{d}{dx} \right) \left(-\frac{i h}{2\pi} \frac{d}{dx} \right) \quad (41)$$

$$K.E = \frac{h^2}{4\pi^2 m} \left(\frac{d^2}{dx^2} \right) \quad (42)$$

See the difference between them

Postulate 3. In any measurement of the observable associated with operator \hat{A} , the only values that will ever be observed are the eigenvalue a , which satisfy the eigenvalue equation

$$\hat{A}\psi = a\psi$$

This postulate captures the central point of quantum mechanics the values of dynamical variables can be quantized (although it is still possible to have a continuum of eigenvalues in the case of unbound states). If the system is in an eigenstate of \hat{A} with eigenvalue a , then any measurement of the quantity A will yield a .

Postulate 4. If a system is in a state described by a normalized wave function, then the average value of the observable corresponding to \hat{A} is given by

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi^* \hat{A} \psi d\tau$$

Postulate 5. The wavefunction or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$H\psi(q,t) = \frac{h}{2i\pi} \cdot \frac{d}{dt} \psi(q,t) \quad (43)$$

Postulate 6. The total wavefunction must be antisymmetric with respect to the interchange of all coordinates of one fermion's with those of another. Electronic spin must be included in this set of coordinates.

The Pauli Exclusion Principle is a direct result of this antisymmetry principle. We will later see that Slater determinants provide a convenient means of enforcing this property on electronic wavefunctions