

The Postulates of Quantum Mechanics

POSTULATE I. The state of a single particle is described as fully as possible by an appropriate state function, $\Psi(x, y, z, t)$, which may be expressed for stationary energy states as the product of a time-independent amplitude function, $\psi(x, y, z)$ and a time-dependent function $f(t)$. Both functions, Ψ and ψ , must be single-valued, continuous, and finite for all values of their coordinates, and must be smoothly varying within the boundaries at which they go to zero.

III

POSTULATE II. a) The possible state functions $\Psi(x, y, z, t)$ for a single particle are given by the solution of the time-dependent Schrödinger wave equation:

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V(x, y, z, t) \right] \Psi = \left[-\frac{\hbar}{i} \left(\frac{\partial}{\partial t} \right) \right] \Psi,$$

b) In the special case of conservative systems, where V is not dependent on t , and $\Psi(x, y, z, t) = \psi(x, y, z)e^{-iEt/\hbar}$, the possible time-independent amplitude functions $\psi(x, y, z)$ for a single particle are given by solution of the time-independent Schrödinger equation,

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V(x, y, z) \right] \psi = E\psi,$$

IV

POSTULATE III. a) For every dynamical variable there is a corresponding linear operator \hat{A} . If the dynamical variable is capable of exact experimental determination, its only possible exact values A are those given by the eigenvalues of the equation

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

b) In the special case of conservative systems and for time-independent operators, the only possible exact values of the dynamical variable are also given by

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

POSTULATE IV. a) The term $|\Psi|^2 dt$ or $\psi^*\psi dz$ is the time-dependent probability that a single particle exists at a given time t in the space element dz , that is, between x, y, z and $(x + dx), (y + dy)$, and $(z + dz)$.

b) For the special case of a conservative system, in which the single particle is restricted to an energy eigenstate, the time-independent probability that the particle exists in the space element dz is $|\psi|^2 dz$ or $\psi^*\psi dz$.

POSTULATE V. a) The expected mean value \bar{A} of a series of measurements of an observable A made over a large number of particles each in the state represented by Ψ is

$$\bar{A} = \frac{\int_{-\infty}^{+\infty} \Psi^* \hat{A} \Psi dz}{\int_{-\infty}^{+\infty} \Psi^* \Psi dz},$$

where \hat{A} is the quantum-mechanical operator for the observable.

b) For the special case of conservative systems in which the operator \hat{A} does not depend explicitly on time,

$$\bar{A} = \frac{\int_{-\infty}^{+\infty} \psi^* \hat{A} \psi dz}{\int_{-\infty}^{+\infty} \psi^* \psi dz}.$$

c) For the special case of conservative systems and time-independent operators and where the wave functions are normalized,

$$\bar{A} = \int_{-\infty}^{+\infty} \psi^* \hat{A} \psi dz.$$

PAULI EXCLUSION PRINCIPLE. To be acceptable, the total wave function for a system of electrons must be antisymmetric to the simultaneous exchange of coordinates and spins between any pair of electrons.