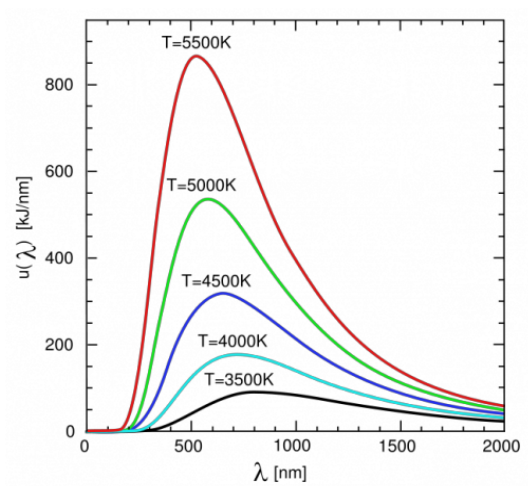
Section 7.3. Basic Concepts and Postulates of Quantum Mechanics

Note. In this section we state several definitions and five postulates for our approach to quantum mechanics.

Note. A *blackbody* is a perfect absorber (and emitter) of radiation. "Since it reflects no light at all, it must appear perfectly black unless it is *emitting* light in the visible region of the spectrum" (page 43 of E. A. Anderson, *Modern Physics and Quantum Mechanics*, W. B. Saunders, 1971). The radiation is emitted with intensity (according to Planck's formula)

$$I(\lambda, T) = \frac{c_1}{\lambda^5}\frac{1}{e^{c_2/(\lambda T)} - 1}$$

where c_1 and c_2 are empirical constants. The graph of $I(\lambda, T)$ for various values of T is:



From `https://www.e-education.psu.edu/astro801/content/l3_p5.html`

(accessed 4/19/2019)

Note. Planck also postulated that energy is not emitted (or absorbed) over a continuum, but instead only in discrete quantities of energy $E = hv = \hbar\omega$ where $h = 6.625 \times 10^{-27}$ erg sec, and $\hbar = h/(2\pi)$.

Note. Classically Rutherford's model of the atom involved electrons orbiting a nucleus. However, according to Maxwell's equation, the electrons should be emitting energies and therefore the orbit would decay and crash into the nucleus. However, if the energy is only radiated in quantum units, this problem is avoided. We now state our first postulate.

Postulate I. (**The State Vector.**)
Every possible state of a given system in quantum mechanics corresponds to a separable Hilbert space over the complex scalar field. A *state* of the system is represented by a nonzero vector in the space, and every nonzero scalar multiple of a state vector represents the same state (and conversely).

Note. The state vector to which the state of the system corresponds at time t is denoted $\psi(x, t)$ and is the *time dependent state vector*. Information about the system can be obtained from the vector $\psi(x, t)$.

Note. We denote a state vector $\psi(x)$ as $\psi(x) = \langle x|\psi\rangle$ and $\overline{\psi(x)} = \langle\psi|x\rangle$. We impose a normalizing condition

$$\int \overline{\psi(x)}\psi(x)\,dx = \int |\psi(x)|^2\,dx = 1$$

or

$$\int \langle\psi|x\rangle\langle x|\psi\rangle\,dx = \int |\langle\psi|x\rangle|^2\,dx = 1.$$

We also denote this as $\langle\psi|\psi\rangle = \langle\psi,\psi\rangle = 1$.

Note. The inner product of two state vectors $|\varphi\rangle$ and $|\psi\rangle$ is

$$\langle\varphi|\psi\rangle - \int \overline{\varphi(x)}\psi(x)\,dx = \int \langle\varphi|x\rangle\langle x|\psi\rangle\,dx.$$

Notice $\langle\varphi|\psi\rangle = \overline{\langle\psi|\varphi\rangle}$.

Definition. State vectors $|\varphi\rangle$ and $|\psi\rangle$ are *orthogonal* if $\langle\varphi|\psi\rangle = 0$. A set $\{|\psi_1\rangle, |\psi_2\rangle, \ldots\}$ is *orthonormal* if $\langle\psi_i|\psi_j\rangle = \delta_{ij}$.

Note. If $\{|\psi_i\rangle\}$ is an orthonormal basis then all state satisfy $|\psi\rangle = \sum_i c_i\,|\psi_i\rangle$ where $c_i = \langle\psi_i|\psi\rangle$. This is the *Principle of Superposition.*

Note. The state vector $\psi(x,t)$ is sometimes called the *wave function.* We will be concerned with the time evolution of ψ.

Postulate II. (**Observable Operators and Their Values**)

(a) To every physical observable, there corresponds in the Hilbert space a Hermitian operation $\hat{A}$ which has a complete set of orthonormal eigenvectors $\{\psi_n\}$ with corresponding eigenvalues $\{\lambda_n\}$ such that $\hat{A}\psi_n = \lambda_n\psi_n$. Conversely, to each such operator there corresponds some physical observable.

(b) The only possible values of a physical observable are the various eigenvalues.

Note. The eigenvalues of $\hat{A}$ are real since $\hat{A}$ is Hermitian. The eigenvalues of the operator can be discrete, continuous, or a combination of the two (see page 350).

Definition. The *commutator* of operators $\hat{A}$ and $\hat{B}$ is $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

Note. Let $\hat{x}$ be the position observable and $\hat{p} = -i\hbar\partial/\partial x$ be the momentum operator. Then

$$[\hat{x}, \hat{p} - \psi = (\hat{x}\hat{p} - \hat{p}\hat{x})\psi - \hat{x}\left(-i\hbar\frac{\partial\phi}{\partial x}\right) - \hat{p}(\hat{x}\psi)$$

$$= -i\hbar\hat{x}\frac{\partial\psi}{\partial x} + i\hbar\left(\psi + x\frac{\partial\psi}{\partial x}\right) = i\hbar\psi$$

and so $[\hat{x}, \hat{p}] = i\hbar$.

Definition. Two observables are *complementary* if their commutator is nonzero. They are *compatible* if the commutator is 0.

Note. Position and momentum are complementary. Momentum $\hat{p} = -i\hbar\partial/\partial x$ and energy $\hat{B} = \hat{T} = (1/(2m))\hat{p}^2 = (-\hbar/(2m))(\partial^2/\partial x^2)$ are compatible:

$$[\hat{p}, \hat{T}]\psi = \left[-i\hbar\frac{\partial}{\partial x}, -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\right]\psi = \left(\frac{-i\hbar^3}{2m}\frac{\partial^3}{\partial x^3} + \frac{i\hbar^3}{2m}\frac{\partial^3}{\partial x^3}\right)\psi = 0.$$

Therefore energy and momentum CAN be determined simultaneously (for a free particle).

Postulate III. (**Correspondence Principle**)

A quantum observable operator corresponding to a dynamical variable is obtained by replacing the canonical variable in classical mechanics by the corresponding quantum mechanical operator.

Note. See page 353 for a list of some operators.

Postulate IV. (**Quantization**)

Every pair of canonically conjugate observable operators (that is, operators dependent classically only on p [momentum] and q [position]) satisfies the following Heisenberg commutation relations:

$$[\hat{q}_m, \hat{q}_n] = 0 = [\hat{p}_m, \hat{p}_n]$$

$$[\hat{q}_m, \hat{p}_n] = i\hbar\hat{\delta}_{mn}$$

where $\hat{q}_m$ is the position operator and $\hat{p}_m$ is the momentum operator.

Note. We now state two more definitions, two theorems without proof, and another postulate.

Definition 7.3.1. The *expectation value* $\langle \hat{A} \rangle$ of an observable operator $\hat{A}$ is the state $\psi(x)$ of a physical system is defined by

$$\langle \hat{A} \rangle = \frac{\langle \psi, \hat{A}\psi \rangle}{(\psi, \psi)} = \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle}.$$

If the state ψ is normalized, then the expectation value is

$$\langle \hat{A} \rangle = (\psi, \hat{A}\psi) = \langle \psi | \hat{A} | \psi \rangle.$$

Definition 7.3.2. The *root-mean-square deviation* is defined by the square root of the expectation value of $(\hat{A} - \langle \hat{A} \rangle)^2$ in the state ψ in which $\langle \hat{A} \rangle$ is computed.

Theorem 7.3.1.

(i) $(\Delta \hat{A})^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$,

(ii) $\langle \hat{A}^2 \rangle = \|\hat{A}\psi\|^2$.

Theorem 7.3.2. A necessary and sufficient condition for a physical system to be an eigenstate of an observable $\hat{A}$ is $\Delta \hat{A} = 0$.

Postulate V. (**Outcome of Quantum Measurement**)
If an observable operator $\hat{A}$ has eigenbasis $\{\psi_n\}$ with the corresponding eigenvalues $\{\lambda_n\}$ then the probability that the measurement will yield the eigenvalue λ_n of $\hat{A}$ is $P(\lambda_n) = |\langle \psi_n | \psi \rangle|^2$ where ψ is normalized.

Note. We wrap up with two more ideas. The first, the Heisenberg Uncertainty Principle, is from Section 7.4 and the second, our final postulate for quantum mechanics (the Schrödinger Equation), is from Section 7.5.

Theorem 7.4.1. The Uncertainty Principle.
If $\hat{A}$ and $\hat{B}$ are Hermitian then

$$\Delta \hat{A} \Delta \hat{B} > \frac{1}{2} \left| \frac{1}{i} \langle [\hat{A}, \hat{B}] \rangle \right|$$

where $\langle [\hat{A}, \hat{B}] \rangle = \langle (\psi, (\hat{A}\hat{B} - \hat{B}\hat{A})\psi) \rangle$.

Note. The Uncertainty Principle implies $\Delta x_j \Delta p_j \geq \hbar/2$.

Postulate VI.

(a) **(Hamiltonian Operator.)** For every physical system ther exists a linear Hermitian operator $\hat{H}$, the *Hamiltonian Operator*, which represents the observable operator corresponding to the total energy of the system.

(b) (Schrödinger's Equation.) If a physical system is not disturbed by any experiment, the Hamiltonian operator $\hat{H}$ determines the time development of the state vector of the system $\Psi(\vec{r}, t)$ through the partial differential equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi(\vec{r}, t).$$

This is called the *time-dependent Schrödinger equation.*

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