Part IV

The Quantum Formalism

From previous lectures

Nature is described by quantum mechanics

- Energy of any system and exchange of energy both are quantized. Their scale is very small because of smallness of Planck's constant h.

- Any system is capable of displaying both particle-like and wave-like properties. Examples are photoelectric effect and diffraction of electrons by periodic potentials.

- Smallness of h makes classical mechanics an excellent approximation at macroscopic scale. For example, energy of a light quantum is of the order of $1 \, \text{eV} \, (10^{-19} \, \text{Joule})$, so that macroscopic energy appears to be varying continuously.

Old quantum theory and the correspondence principle

- In old quantum mechanics (semiclassical theory), quantum condition is given by quantization of action for periodic motion. It leads to quantization of energy. The theory mixes classical and quantum pictures.

- Correspondence principle demands that quantum results go to classical results at large values of quantum numbers, providing a link between quantum and classical results.

Quantum Mechanics developed by Heisenberg and Schrödinger

- Quantum mechanics describes a system in terms of only observable quantities. Thus position of an electron or its momentum have no direct meaning. These are represented by the frequency and the corresponding amplitude that gives the intensity of light emitted at that frequency.

- All possible frequencies ω_{mn} and amplitudes X_{mn} are needed for a complete quantum mechanical description of the system. This is exactly like in classical physics where the position of particle performing periodic motion for energy E is given as $x_E(t) = \sum_\tau X_{E,\tau} e^{i\tau\omega t} + X_{E,-\tau} e^{-i\tau\omega t}$.

- Wave mechanics describes a system in terms of its wavefunction $\psi(x,t)$. The wavefunction and its time evolution is determined by the Schrödinger equation $i\frac{\partial\psi}{\partial t} = H\psi$.

Born interpretation of the wavefunction

- Probability density (probability per unit length in one dimension) is given by the square of the absolute value $|\psi(x)|^2$ of the wavefunction $\psi(x)$.
- So, probability of finding a particle between x and $x + \Delta x$ is

$$|\psi(x)|^2 \Delta x$$

Operators give matrix elements and average values of x and p

- Operator for position x is a multiplicative operator

$$\hat{x}\psi(x) = x\psi(x)$$

$$x_{mn} = \int \psi_m^*(x)\, x\, \psi_n(x)dx \qquad \langle x \rangle = \int \psi^*(x)\, x\, \psi(x)dx$$

- Operator for x component of momentum p_x is a differential operator

$$\hat{p}_x\psi(x) = \frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}$$

$$(p_x)_{mn} = \int \psi_m^*(x)\frac{\hbar}{i}\frac{\partial\psi_n(x)}{\partial x}dx \qquad \langle p_x \rangle = \int \psi^*(x)\frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}dx$$

Operators for other quantities are obtained from operators for x and p

- **Operator for square of momentum and its expectation value**

$$\hat{p}_x^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \qquad \langle p_x^2 \rangle = -\hbar^2 \int \psi^*(x) \frac{\partial^2 \psi(x)}{\partial x^2}$$

- **Kinetic energy (KE) operator and its expectation value**

$$\frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \qquad \langle KE \rangle = -\frac{\hbar^2}{2m} \int \psi^*(x) \frac{\partial^2 \psi(x)}{\partial x^2}$$

- **Operator for energy is the Hamiltonian**

$$\hat{H} = KE + PE = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

- **The Schrödinger equation (time-dependent and stationary state)**

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi \qquad\qquad \hat{H}\psi = E\psi$$

Lecture 23

Completing quantum formalism
&
The Copenhagen Interpretation

Operators for observables and their eigenvalues and eigenfunctions

- For each operator $\widehat{O}$ corresponding to an observable, there is an eigenvalue equation

$$\widehat{O}\psi_\alpha(x) = O_\alpha \psi_\alpha(x)$$

  with eigenvalue O_α. The eigenvalue O_α is a real number.

- Eigenfunctions belonging to different eigenvalues are orthogonal.

- **Meaning of eigenvalue:** When measurement of an observable is made on a system - (i) the result is one of the eigenvalues of the corresponding operator $\widehat{O}$ and (ii) the system wavefunction becomes the corresponding eigenfunction.

- Thus if energy of a system is measured, outcome will be one of the energy eigenvalues of the Schrödinger equation $\widehat{H}\psi_E = E\psi_E$.

Eigenfunctions for position and momentum operators

- For position operator the eigenfunction with position eigenvalue x_0 is

$$\psi_{x_0}(x) = \delta(x - x_0)$$

  since

$$\widehat{x}\boldsymbol{\psi}_{\boldsymbol{x_0}}(\boldsymbol{x}) = \hat{x}\delta(x - x_0) = x\delta(x - x_0) = x_0\delta(x - x_0) = \boldsymbol{x_0}\boldsymbol{\psi}_{\boldsymbol{x_0}}(\boldsymbol{x})$$

- Eigenfunction for the momentum operator with eigenvalue p_0 is

$$\psi_{p_0}(x) = Ae^{ip_0x/\hbar}$$

  because

$$\widehat{p}\boldsymbol{\psi}_{\boldsymbol{p_0}}(\boldsymbol{x}) = \frac{\hbar}{i}\frac{\partial}{\partial x}Ae^{ip_0x/\hbar} = p_0Ae^{ip_0x/\hbar} = \boldsymbol{p_0}\boldsymbol{\psi}_{\boldsymbol{p_0}}(\boldsymbol{x})$$

Summary and comments:

- If a system is not in one of the eigenstates of an observable, a measurement of the observable gives one of its eigenvalues and the system wavefunction becomes the associated eigenfunction.

- If a system is in one of the eigenstates of an observable, repeated measurements will keep giving the same eigenvalue.

- Only if a system is in an eigenstate of the Hamiltonian (energy), $|\psi(x,t)|^2$ is independent of time.

- If a system initially is in a state that is an eigenstate of some operator but not an eigenstate of energy, $|\psi(x,t)|^2$ will keep on changing with time with $\psi(x,t)$ determined by time-dependent Schrodinger equation.

- If $\psi(x, t = 0) = \sum_c C_n \psi_n(x)$ then $\psi(x,t) = \sum_c C_n \psi_n(x) e^{-iE_n t/\hbar}$. Here $\psi(x, t = 0)$ is normalized. It is easy to see that $\psi(x,t)$ then remains normalized.

Eigenfunctions of an observable form a complete set

- **Meaning of complete set:** Any function $f(x)$ satisfying the same boundary condition as the functions $\{\psi_n(x)\}$ in a set can be expanded in terms of these functions as $f(x) = \sum_n C_n \psi_n(x)$ or $\sum_m \psi_n^*(x')\psi_n(x) = \delta(x - x')$.

- if some functions other than those from the set $\{\psi_n(x)\}$ were required to be added to the series $f(x) = \sum_n C_n \psi_n(x)$, measuring the value of the corresponding observable when system has wavefunction $f(x)$ will sometimes give a value other than one of the eigenvalues. But the measurement always gives one of all the eigenvalues so the series contains no function other than $\{\psi_n(x)\}$. These functions are thus sufficient to write $f(x) = \sum_n C_n \psi_n(x)$ with $C_n = \int \psi_n^*(x)f(x)dx$. That shows completeness of $\{\psi_n(x)\}$ on the basis of physics arguments.

Examples: expanding a function in terms of different eigenfunctions

- Position eigenfunctions

$$f(x) = \sum_{x_0} f(x_0)\delta(x - x_0) = \int f(x_0)\delta(x - x_0)dx_0$$

$$f(x_0) = \int f(x)\delta(x - x_0)dx$$

- Momentum eigenfunctions

$$f(x) = \sum_p C_p e^{ipx/\hbar} = \int C(p)e^{ipx/\hbar}dp$$

$$C(p) = \int f(x)e^{-ipx/\hbar}dx$$

- Energy eigenfunctions (*you have shown completeness in terms of Dirac delta function in one of the Assignment problems*)

$$f(x) = \sum_c C_n\psi_n(x) \qquad C_n = \int \psi_n^*(x)f(x)dx$$

What do the coefficients C_n in the expansion $f(x) = \sum_n C_n \psi_n(x)$ mean physically?

- Consider a large number of copies of a system with wavefunction $\psi(x) = f(x) = \sum_n C_n \psi_n(x)$ formed by superposing eigenfunctions $\{\psi_n(x)\}$ of an operator $\widehat{O}$.

- Measuring the observable corresponding to $\widehat{O}$ on each these copies will give the set of eigenvalues $\{O_\alpha\}$ from which the average value of the observable for the wavefunction $\psi(x)$ can be calculated. This is the expectation value of the operator $\widehat{O}$ and its value is

$$\langle \widehat{O} \rangle = \sum_n \text{probability of system being in state n} \times O_n$$

What do the coefficients C_n mean ....?

- On the other hand

$$\langle \widehat{O} \rangle = \int \psi^*(x) \widehat{O} \psi(x) dx = \sum_n |C_n|^2 O_n$$

(Here we have used the condition that $\int \psi_m^*(x) \psi_n(x) dx = \delta_{mn}$)

- This gives

Probability of finding the system in eigenstate n of $\widehat{O}$ while mesuring the corresponding observable $= |C_n|^2$

- Note that because of normalization of $\psi(x)$, we must have

$$\sum_n |C_n|^2 = 1$$

Copenhagen interpretation of Quantum Mechanics
Reference: "A student's Guide to Schrodinger Equation" by Daniel A. Fleisch

- *Information Content*   The quantum state Ψ has all possible information about a system.

- *Time evolution* Over time, quantum states evolve smoothly in accordance with the Schrodinger equation unless a measurement is a made.

- *Wavefunction collapse*   Whenever a measurement of a quantum state is made, the state **collapses** to an eigenstate of the operator associated with the observable being measured.

- *Measurements results* The value measured for an observable is the eigenvalue.

Copenhagen interpretation…………

- **_Uncertainty principle_** Certain observable (such as position and momentum in the same direction may not be simultaneously known with arbitrary great precision.

- **_Born rule_** The probability that a quantum state will collapse to a given eigenstate upon measurement is determined by the square of the amount of that eigenstate present in the original state (the wavefunction).

- **_Correspondence principle_** In the limit of very large quantum numbers, the results of measurements of quantum observables must match the results of classical physics.

- **_Complementarity_** Every quantum state includes complementary wave-like and particle-like aspects; whether a system behaves like a wave or like a particle when measured is determined by the nature of measurement.

An example: Measurement of momentum when a particle is in the ground-state of a simple harmonic oscillator

- The wavefunction

$$\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} = C \int dp\, e^{-\sigma p^2} e^{ipx/\hbar} = \int C_p \psi_p(x)\, dp$$

- Probability of finding momentum between p_0 and $p_0 + \Delta p$

$$|C|^2 e^{-2\sigma p^2} \Delta p$$

- Expectation value of the momentum

$$\langle p \rangle = \int dp\, p\, |C|^2 e^{-2\sigma p^2}$$

An example: Measurement of momentum ……….

- **Wavefunction collapse:** If the momentum of the particle is measured to be p_0 , then immediately after the measurement, the particle will have the wavefunction $\psi(x) = e^{ip_0 x/\hbar}$.

- Therefore its energy will be uncertain because

$$e^{ip_0 x/\hbar} = \sum_n C_n \psi_n(x)$$

- And the wavefunction will evolve with time as

$$\psi(x, t) = \sum_n C_n \psi_n(x) \, e^{-iE_n t/\hbar}$$