The Postulates of Quantum Mechanics

Part I

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Introduction

Introduction: Classical Mechanics

- In Classical Mechanics, the motion of any physical system is determined if the position $[\vec{r}(x, y, z)]$ and the velocity $[\vec{v}(\dot{x}, \dot{y}, \dot{z})]$[1] of each of its points are known as a function of time
- In general, to describe such a system one introduces the following coordinates:
  Generalized coordinates

$$q_i(t)(i = 1, 2, ..., N)$$

  Generalized velocities

$$\dot{q}_i(t)(i = 1, 2, ..., N)$$

- Specifying $q_i(t)$ and $\dot{q}_i(t)$ enables us to calculate, at any given instant, the position and velocity of any point of the system.

[1] Where $\rightarrow \dot{} \equiv \frac{d}{dt}$

Introduction: Classical Mechanics

- Using the Lagrangian $\mathcal{L}(q_i, \dot{q}_i, t)$, one defines the conjugate momentum p_i of each of the generalized coordinates q_i

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$$

where $q_i(t)$ and $p_i(t)$ are fundamental dynamical variables. All physical quantities associated with the system (energy, angular momentum, etc) can be expressed in terms of them.

Exemplo: The total energy of the system is given by the classical Hamiltonian $\mathcal{H}(q_i, p, t)$

The motion of the system can be studied by using either Lagrange's equation or the Hamilton-Jacobi canonical equations:

$$\frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}$$

$$\frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}$$

◇ If the forces acting on a particle of mass m can be derived from a scalar potential $V(\vec{r},t)$, the Hamiltonian is:

$$\mathcal{H}(\vec{r},\vec{p},t) = \frac{p^2}{2m} + V(\vec{r},t).$$

The Hamilton-Jacobi Equations (HJE) take the form:

$$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m}, \quad \frac{d\vec{p}}{dt} = -\nabla V$$

The classical description of a system can be summarized as follows

(i) The state of the system at a fixed time t is defined by specifying N generalized $q_i(t_0)$ and their N conjugate momentum $p_i(t_0)$

(ii) The value, at a given t, of the physical quantities is determined when the state of the system at this time is known: knowing the state of the system, one can predict with certain the result of any measurement performed at time t_0

(iii) The time evolution of the state of the system is given by the HJE: they are first-order differential equations, and their solution $\{q_i(t), p_i(t)\}$ is unique if the value of these functions at a given time t_0 is fixed, and the state of the system is known for all time if its initial state is known

In the following lectures, we will study the postulates on which the quantum description of the physical systems is based

The postulates will provide us with the 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 measurement results of physical quantities?**

(iii) **How can the system's state at a time t be found when the state at a time t_0 is known?**

Quantum Mechanics: Example 1

Free Particle

- Ψ) Let's analyze more carefully the concept of the quantum state of a particle
- Ψ) To illustrate this, let's consider the example of a free particle

Consider a particle whose potential energy is zero at every point in space. The particle is thus not subject to any force. In this case, it is said to be free.

FREE PARTICLE

Ψ) We have discussed in previous lectures that when the particle of mass m is subjected to the influence of a potential $V(\vec{r}, t)$, the Schrödinger equation takes the form:

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) + V(\vec{r}, t)\psi(\vec{r}, t). \tag{1}$$

This equation is linear and homogeneous in ψ. For the case $V = 0$:

$$i\hbar \frac{\partial \psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t). \tag{2}$$

These equations are satisfied by solutions of the form (See pre-req. lectures)

$$\psi(\vec{r}, t) = Ae^{i(\vec{k}.\vec{r} - wt)} \tag{3}$$

where A is a constant.

Free Particle

where A is a constant, and

$$w = \frac{\hbar k^2}{2m}. \tag{4}$$

According to de Broglie relations, $E = h\nu = \hbar w$ and $\vec{p} = \hbar\vec{k} \Rightarrow \lambda = \frac{2\pi}{|\vec{k}|} = \frac{h}{|\vec{p}|}$.

Eq. (4) expresses the fact that the energy E and momentum $\vec{p}$ of a free particle satisfy the equation, which is well-known in Class. mechanics: $E = \frac{p^2}{2m}$. Since $|\psi(\vec{r}, t|^2 = |A|^2$.

A plane wave of this type represents a particle whose probability of presence is uniform throughout all space

Free Particle

Ψ) The principle of superposition tells us that every linear combination of a plane wave satisfying Eq. (4) will also be a solution of the Schrödinger equation. Such superposition can be written:

$$\psi(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \int g(\vec{k}) e^{i(\vec{k}.\vec{r} - w(k)t)} d^3k \tag{5}$$

$d^3k \longrightarrow$ infinitesimal volume element in k-space $\Rightarrow d^3k = dk_x dk_y dk_z$.

$g(\vec{k}) \longrightarrow$ can be complex and must be sufficiently regular to allow differentiation inside the integral

Ψ) It can be shown that any square-integrable solution can be written in the form of Eq. (5).

Ψ) A wave function such as Eq. (5), a superposition of plane waves, is called a three-dimensional ”wave packet”.

Free Particle

Ψ) For the sake of simplicity, let's consider a one-dimensional wave packet propagating in the x direction

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}} \int g(k) e^{i(kx - w(k)t)} dk \tag{6}$$

Ψ) We are interested in the form of the wave packet at a given instant, $t = t_0 = 0$

$$\psi(x,0) = \frac{1}{(2\pi)^{1/2}} \int g(k) e^{i(kx)} dk \tag{7}$$

we see that $g(k)$ is the Fourier transform

$$g(k) = \frac{1}{(2\pi)^{1/2}} \int \psi(x,0) e^{-i(kx)} dx \tag{8}$$

FREE PARTICLE

- Ψ) Consequently, the validity of Eq. (7) is not limited to the case of the free particle (whatever $\psi(x,0)$ can be written in this form).
- Ψ) The form of the wave packet is given by the x-dependence of $\psi(x,0)$ defined by Eq. (7).
- Ψ) Let us illustrate this by one example:

Now, imagine $g(k)$ with a peak at $k = k_0$ and width Δk. Consider too that $\psi(x,0)$ instead of being the superposition of an infinite number of plane waves as in Eq. (7), be the sum of only three waves, with $k_1 = k_0, k_2 = k_0 - \Delta k/2, k_3 = k_0 + \Delta k/2$. Then we have:

$$\begin{aligned}\psi(x) &= \frac{g(k_0)}{\sqrt{2\pi}}\left[e^{ik_0x} + \frac{1}{2}e^{i(k_0-\Delta k/2)x} + \frac{1}{2}e^{i(k_0+\Delta k/2)x}\right] \\ &= \frac{g(k_0)}{\sqrt{2\pi}}e^{ik_0x}\left[1+\cos\left(\frac{\Delta k}{2}x\right)\right]\end{aligned} \tag{9}$$

Free Particle

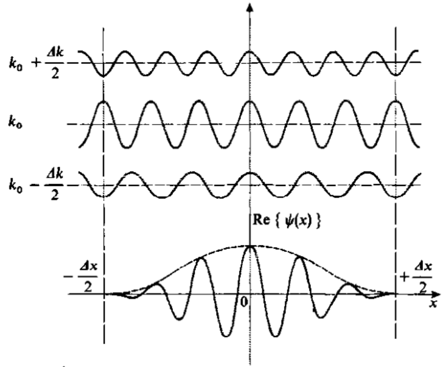

FIGURE 4

The real parts of the three waves whose sum gives the function $\psi(x)$ of (C-10). At $x = 0$, the three waves are in phase and interfere constructively. As one moves away from $x = 0$, they go out of phase and interfere destructively for $x = \pm \Delta x/2$.

In the lower part of the figure, Re $\{ \psi(x) \}$ is shown. The dashed-line curve corresponds to the function $\left[1 + \cos\left(\frac{\Delta k}{2}x\right)\right]$, which, according to (C-10), gives $|\psi(x)|$ (and therefore, the form of the wave packet).

Quantum Mechanics: Example 2

Particle in a Time-Independent Scalar Potential

Stationary states

Ψ) The wave function of a particle whose potential energy $V(\vec{r})$ is time-independent must satisfy the Schrödinger equation

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V(\vec{r})\psi(\vec{r},t) \tag{10}$$

Ψ) Let's see if there exist solutions to this equation (i.e. if there exist stationary states) of the form: $\psi(\vec{r},t) = \varphi(\vec{r})\chi(t)$

Inserting this one in Eq. (10) and then dividing both sides by the product $\varphi(\vec{r})\chi(t)$

$$\frac{i\hbar}{\chi(t)}\frac{d\chi(t)}{dt} = -\frac{\hbar^2}{2m\varphi(\vec{r})}\nabla^2\varphi(\vec{r}) + V(\vec{r}) \tag{11}$$

Particle in a Time-Independent Scalar Potential

- Ψ) This equation equates a function t on the (LHS and a function of $\vec{r}$ on the RHS
- Ψ) This equality is only possible if each of these functions is a constant, which we set to[2]: $\hbar w$
- Ψ) Setting the LHS equal to $\hbar w$, we obtain for $\chi(t)$ a differential equation of the form:

$$i\hbar \frac{1}{\chi(t)} \frac{d\chi(t)}{dt} = \hbar w \tag{12}$$

with solution,

$$\chi(t) = A e^{-iwt} \tag{13}$$

[2]we need a dimension of $\hbar$ over time, w must have a dimension of angular frequency (we know we are dealing with waves)

Particle in a Time-Independent Scalar Potential

Ψ) In the same way, $\varphi(\vec{r})$ must satisfy the equation:

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\vec{r}) + V(\vec{r})\varphi(\vec{r}) = \hbar w\varphi(\vec{r}) \tag{14}$$

as $\psi(\vec{r},t) = \varphi(\vec{r})\chi(t)$

$$\psi(\vec{r},t) = \varphi(\vec{r})Ae^{-iwt} = \varphi(\vec{r})e^{-iwt} \tag{15}$$

where we incorporate the constant A into $\varphi(\vec{r})$.

A wave function of the form of Eq. (15) is called: A stationary solution of the Schorödinger equation.

It leads to time a time-independent probability density

$$\psi^*\psi = |\psi(\vec{r},t)|^2 = |\varphi(\vec{r})|^2 \tag{16}$$

Particle in a Time-Independent Scalar Potential

- Ψ) In a stationary function, only one angular frequency (w) appears. According to the Planck-Einstein relations, a stationary state is a state with well-defined energy: $E = \hbar w = \hbar \nu$
- Ψ) In Classical Mechanics, when a potential energy is time-independent, the total energy is a constant of motion
- Ψ) In Quantum Mechanics, there exists a well-determined energy state, and Eq. (14) can be written as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\varphi(\vec{r}) = E\varphi(\vec{r}) \Rightarrow H\varphi(\vec{r}) = E\varphi(\vec{r}) \qquad (17)$$

where H is a differential operator: $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$.

H is a linear operator, thus, if λ_1 and λ_2 are constants, we have

Particle in a Time-Independent Scalar Potential

$$H\left[\lambda_1\varphi_1(\vec{r}) + \lambda_2\varphi_2(\vec{r})\right] = \lambda_1 H\varphi_1(\vec{r}) + \lambda_2 H\varphi_2(\vec{r}) \tag{18}$$

The equation above is the eigenvalue equation of the linear operator H.

We will see in the future that this equation has square integrable solutions for $\varphi(\vec{r})$ only for certain values of $E \to E_n$, which is the origin of energy quantization.

Particle in a Time-Independent Scalar Potential

Ψ) To distinguish between the various possible values of energy E and the corresponding wave functions of $\varphi(\vec{r})$, we label them with an index n. Thus we have, $H\varphi_n(\vec{r}) = E_n\varphi_n(\vec{r})$.

and the stationary states of the particle have wave functions: $\psi_n(\vec{r}, t) = \varphi_n(\vec{r})e^{-iE_nt/\hbar}$.

Ψ) $\psi_n(\vec{r}, t)$ is a solution of the Schrödinger equation.

Ψ) Since it is linear, it has a whole series of other solutions of the form:

$$\psi(\vec{r}, t) = \sum_n c_n\psi_n(\vec{r}, t) = \sum_n c_n\varphi_n(\vec{r})e^{-iE_nt/\hbar} \tag{19}$$

where c_n are arbitrary complex constants.

Particle in a Time-Independent Scalar Potential

In particular, we have

$$\psi_n(\vec{r},0) = \sum_n c_n \varphi_n(\vec{r}) \tag{20}$$

Ψ) Then, assume that we know $\psi(\vec{r},0)$, that is the state of the particle at $t=0$. We will see during the course that any function $\psi(\vec{r},0)$ can always be decomposed in terms of the eigenfunctions of H as in Eq. (20).

Ψ) The coefficients c_n are therefore determined by $\psi(\vec{r},0)$ and the corresponding $\psi(\vec{r},t)$ is then given by Eq. (19).

Ψ) All we need to do to obtain it is to multiply each term of Eq. (20) by the factor: $e^{-iE_n t/\hbar}$. Where E_n is the eigenvalue associated with $\varphi_n(\vec{r})$.

Ψ) We stress the fact that these phase factors differ from one term to another. It is only in the case of stationary states that the t-dependence involves only one exponential.

State of the system

The postulates of quantum mechanics: Description of the state of a system

- Ψ) So, we introduced the concept of a quantum state of a particle;
- Ψ) We characterized this state at a given time (t_0) by a square-integrable wave function;
- Ψ) We can associate a ket of the state space $\mathcal{E}_r$ with each wave function

$$\int d^3r|\psi(\vec{r},t)|^2 = 1 \tag{21}$$

  where the integration extends over all space. We call this L^2 and it has the structure of a Hilbert space.
- Ψ) Physically we are interested only on $\psi(\vec{r},t)$ that are everywhere defined, continuous, and differentiable.
- Ψ) Let's call $\mathcal{F}$ the set of wave functions composed of sufficiently regular functions of L^2 (i.e. $\mathcal{F}$) is a subspace of L^2

The postulates of quantum mechanics: Description of the state of a system

- Ψ) However, $\psi(\vec{r}, t)$ can be represented by several distinct sets of components, each one corresponding to the choice of a basis.
- Ψ) Since each quantum state of a particle is characterized by a state vector $(\mathcal{E}_r)$. Let's call it the state space of a particle
- Ψ) The fact that the space $\mathcal{F}$ is a subspace of L^2 means that $\mathcal{E}_r$ is a subspace of the Hilbert space.
- Ψ) Choosing $|\psi\rangle$ belonging to $\mathcal{E}_r$ is equivalent to choosing the function:$\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$.
- Ψ) Therefore, the quantum state of a particle at a fixed time is characterized by a ket of the space $\mathcal{E}_r$
- Ψ) In this form, the concept of a state can be generalized to any physical system

Homework: Examples in Complement H_I (page 67)

The postulates of quantum mechanics: Description of the state of a system

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 $\mathcal{E}$

THE POSTULATES OF QUANTUM MECHANICS: DESCRIPTION OF THE STATE OF A SYSTEM

- Ψ) It is important to note that, since $\mathcal{E}$ is a vector space;
- Ψ) This first postulate implies a superposition principle: a linear combination of a state vector is a state vector

Example: Quantum computing

- Ψ) The simplest quantum mechanical system is the qubit. It has a two-dimensional state space
- Ψ) Suppose $|0\rangle$ and $|1\rangle$ form an orthonormal basis for that state space
- Ψ) An arbitrary state vector in the state space can be written as:

$$|\psi\rangle = a|0\rangle + b|1\rangle$$

a and b are complex numbers that satisfy $|a|^2 + |b|^2 = 1$ as a consequence of the condition $\langle\psi|\psi\rangle = 1$. Then, $|\psi\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$

Physical quantities

The postulates of quantum mechanics: Description of physical quantities

Ψ) We have seen in the examples above a differential operator H related to the total energy of a particle in a scalar potential

Ψ) This is simply a special case of the following (second) postulate:

The postulates of quantum mechanics: Description of physical quantities

Second Postulate: Every measurable physical quantity $\mathcal{A}$ is described by an operator A in $\mathcal{E}$. This operator is an observable.

The postulates of quantum mechanics: Description of physical quantities

Ψ) Unlike Classical Mechanics, Quantum Mechanics describes in a fundamentally different manner the state of a system and associated physical quantities:

A State is represented by a vector: $|\psi\rangle, [|0\rangle, |1\rangle]$ (qubit notation), etc

A physical quantity by an operator: H (Hamiltonian), H (Hadamard gate), etc

Measurements

The postulates of quantum mechanics: the measurement of physical quantities

$\Psi)$ The connection between the operator H and the particle's total energy that appeared in the examples above can be summarized in the following form:

$\Psi)$ the only possible energies are the eigenvalues of the operator H. Here as well, this relation can be extended to all physical quantities.

The postulates of quantum mechanics: The measurement of physical quantities

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

The postulates of quantum mechanics: The measurement of physical quantities

Ψ) A measurement of $\mathcal{A}$ always give a real value, since A is by definition Hermitian.

Ψ) If the spectrum of A is discrete, the results that can be obtained by measuring $\mathcal{A}$ are quantized.

Example: Suppose $|\psi\rangle = a|0\rangle + b|1\rangle$. Then the probability of obtaining measurement outcome 0 is $|a|^2$.