Notes of Quantum Mechanics

Wyant College of Optical Sciences
University of Arizona

Nicolás Hernández Alegría

Preface

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Contents

List of Figures

List of Tables

Listings

Chapter 1

Postulates of Quantum Mechanics

1.1 Introduction

In classical mechanics, the motion of any physical system is determined through the position $\boldsymbol{r} = (x, y, z)$ and the velocity $\boldsymbol{v} = (\dot{x}, \dot{y}, \dot{z})$. One usually introduces generalized coordinates $q_i(t)$ whose derivatives with respect to time $\dot{q}_i(t)$. are the generalized velocities. With these coordinates, the position and velocity of any point can be calculated. Using the Lagrangian $\mathcal{L}(q_i, \dot{q}_i, t)$ one defines the conjugate momentum p_i os each of the generalized cooridnates q_i:

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

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

The motion (evolution) of a system can be studied by Lagrange's equations or the Hamilton-Jacobi canonical equation:

$$\text{Hamilton-Jacobi equations} \qquad \frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \text{and} \quad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}.$$

The classical description of a physical system can be summarized as follows:

- The state of the system at time t_0 is defined by specifying N generalized coordinates $q_i(t_0)$ and their N conjugate momenta $p_i(t_0)$.
- Knowing the state of the system at t_0, allows to predict with certainty the result of any measurement performed at time t_0.
- The time evolution of the state of the system is given by the **Hmailton-Jacobi** equations. The state of the system is known for all time if its initial state is known.

1.2 Statements of the postulates

1.2.1 State and measurable physical quantites of a system

The quantum state of a particle at a fixed time is characterized by a ket of the space $\mathscr{E}_{\boldsymbol{r}}$.

First postulate: Sate of a system

At time t_0, the state of an isolated physical system is defined by specifying a ket $|\psi(t_0)\rangle \in \mathscr{E}_{\boldsymbol{r}}$.

Recall that, sinsce $\mathscr{E}$ is a vector space, a linear combination of state vectors is a state vector.

Second postulate: Measurable physical quantities

Every measurable physical quantity $\mathcal{A}$ is described by an operator A acting in $\mathscr{E}$: this operator is an **observable**.

In this sense, a state is represented by a vector, while a physical quantity by an operator.

Third postulate: Outcomes of measurements

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

- A measurement of $\mathcal{A}$ gives **always** a real value, since A is Hermitian by definition.
- If the spectrum of A is discrete, the results that can be obtained by measuring $\mathcal{A}$ are **quantized**.

1.2.2 Principle of spectral decomposition

Consider a system whose state is characterized, at a given time, by $|\psi\rangle$, which is assumed normalized. We want to predict the result of the measurement, at thi time, of a physical quantity $\mathcal{A}$ associated with the observable A.

Discrete spectrum

If all eigenvalues a_n of A are non-degenerate, there is associated with each of them a **unique** eigenvector $|u_n\rangle$. As A is an observable, the set of $|u_n\rangle$ which we assume normalized, conssitutes a basis in $\mathscr{E}$ and we can expand $|\psi\rangle$:

$$A|u_n\rangle = a_n|u_n\rangle \Longrightarrow |\psi\rangle = \sum_n c_n|u_n\rangle$$

The probability $P(a_n)$ of finding a_n when $\mathcal{A}$ is measured is therefore:

$$P(a_n) = |c_n|^2 = |\langle u_n|\psi\rangle|^2.$$

If, however, some of the eigenvalues a_n are degenerate, several orthonormalized eigenvectors $|u_n^i\rangle$ corresponds to them and we can still expand $|\psi\rangle$ on the orthonormal basis $\{|u_n^i\rangle\}$:

$$A|u_n^i\rangle = a_n|u_n^i\rangle,\ i = 1, 2, \cdots, g_n \Longrightarrow |\psi\rangle = \sum_n \sum_{i=1}^{g_n} c_n^i|u_n^i\rangle. \tag{1.1}$$

The probability now becomes

$$P(a_n) = \sum_{i=1}^{g_n} |c_n^i|^2 = \sum_{i=1}^{g_n} |\langle u_n^i|\psi\rangle|^2.$$

Foruth postulate (discrete case): Result of a measurement

When $\mathcal{A}$ is measured on a system in the normalized state $|\psi\rangle$, the probability $P(a_n)$ of obtaining the eigenvalue a_n of the observable A is proportional to the projection of ψ onto the eigensubspace $\mathscr{E}_n$:

$$\boxed{P(a_n) = |P_n|\psi\rangle|^2 = \sum_{i=1}^{g_n} |\langle u_n^i|\psi\rangle|^2}\ , \quad g_n = \text{degree of degeneracy of } a_n.$$

$\{|u_n^i\rangle\}$ is a set of orthonormal vectors which forms a basis in the eigensubspace $\mathscr{E}_n$.

Continuous case

If now the spectrum of A is continuous and non-degenerate, the eigenvectors of A forms a continuous basis in $\mathscr{E}$, in terms of which $|\psi\rangle$ can be expanded:

$$A|v_\alpha\rangle = \alpha|v_\alpha\rangle \Longrightarrow |\psi\rangle = \int d\alpha\, c(\alpha)|v_\alpha\rangle.$$

In this case, we cannot define the probability on a single point; we must define a probability density function. The differential probability of obtaining a value included betwen α and $\alpha + d\alpha$ is

$$dP(\alpha) = \rho(\alpha)d\alpha, \quad \text{with} \quad \rho(\alpha) = |c(\alpha)|^2 = |\langle v_\alpha|\psi\rangle|^2.$$

Fourth postulate (continuous case, non-degenerate): Result of a measurement

If $\mathcal{A}$ is measured in the normalized state $|\psi\rangle$, the probability $dP(\alpha)$ of obtaining a result included betwen α and $\alpha + d\alpha$ is

$$dP(\alpha) = |\langle v_\alpha|\psi\rangle|^2\, d\alpha\,. \tag{1.2}$$

In cases where the state $|\psi\rangle$ is **not normalized**, we then use the following expressions:

$$\begin{array}{ll} \text{Discrete case} & \text{Continuous case} \\ P(a_n) = \dfrac{1}{\langle\psi|\psi\rangle}\displaystyle\sum_{i=1}^{g_n}|c_n^i|^2 & \rho(\alpha) = \dfrac{1}{\langle\psi|\psi\rangle}|c(\alpha)|^2. \end{array} \tag{1.3}$$

On the other hand, two proportional state vectors, $|\psi'\rangle = ae^{i\theta}|\psi\rangle$, represent **the same** physical state:

$$|\langle u_n^i|\psi'\rangle|^2 = |e^{i\theta}\langle u_n^i|\psi\rangle|^2 = |\langle u_n^i|\psi\rangle|^2.$$

a is simplified when dividing by $\langle\psi'|\psi'\rangle$.

Global versus relative phase factor

A global phase factor does not affect the physical preditions, but the relative phases of the coefficients of an expansion are significant.

1.2.3 Reduction of the wave packet

We want to measure at a given point the physical quantity $\mathcal{A}$. If the ket $|\psi\rangle$ before the measurement is knwon, the fourth postulate allows us to predict the probability of the various possible outcomes. Immbediately after the measurement, we cannot speak of probability, as we have alreade got the result (collapse).

If the measurement of $\mathcal{A}$ resulted in a_n (assuming discrete spectrum of A), the state of the system immediately after this measurement is the eigenvector $|u_n\rangle$ associate with a_n:

$$\text{State of collapse} \qquad |\psi\rangle \overset{(a_n)}{\Longrightarrow} |u_n\rangle. \tag{1.4}$$

- If we perform a second measurement of $\mathcal{A}$ immediately after the first one, we shall always find the same result a_n.

- We use just after the measurement to assume the system had not time to evolve, because otherwise the state evolves and we need the sixth postulate to keep track of this motion.

When the eigenvalue a_n is degenerate, then the state just before the measurement is written as (equation (1.1)):

$$|\psi\rangle = \sum_n \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle.$$

And the state of collapse just after the measurement is

$$|\psi\rangle \overset{(a_n)}{\Longrightarrow} \frac{1}{\sqrt{\sum_{i=1}^{g_n} |c_n^i|^2}} \sum_{i=1}^{g_n} c_n^i |u_n^i\rangle. \tag{1.5}$$

The square root factor is the normalization so that we get a unitary norm of the state. We rewrite the above expression in the following fifth postulate.

Firfth postulate: State of collapse

If the measurement of the $\mathcal{A}$ in the state $|\psi\rangle$ gives the result a_n, the state of the system immediately after the measurement is the normalized projection of $|\psi\rangle$ onto the eigensubspace $\mathscr{E}_n$ associated with a_n:

$$|\psi\rangle \overset{(a_n)}{\Longrightarrow} \frac{P_n|\psi\rangle}{\sqrt{\langle\psi|P_n|\psi\rangle}} \tag{1.6}$$

It is not an arbitrary ket of $\mathscr{E}_n$, but the part of $|\psi\rangle$ that belongs to $\mathscr{E}_n$.

1.2.4 Time evolution of Systems

Sixth postulate: Time evolution of the system

The time evolution of the state vector $|\psi(t)\rangle$ is governed by the Schrodinger equation:

$$ih\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle\ , \tag{1.7}$$

where $H(t)$ is the **Hamiltonian operator** (observable) associated with the total energy of the system.

1.2.5 Quantization rules

We will discuss how to construct, for a physical quantity $\mathcal{A}$ already deffined in classical mechanics, the operator A which rescribes it in quantum mechanics.

1.3 The physical interpretation of the postulates

1.3.1 Quantization rules are cnsistent with probabilistic interpretation

1.3.2 The measurement process

1.3.3 Mean value of an observable in a given state

1.3.4 The root mean square deviation

1.3.5 Compatibility of observables

1.4 Physical implications of the Schrodinger equation

Recall the Schrodinger equation

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi\rangle. \tag{1.8}$$

1.4.1 General properties of the Schrodinger equation

The ir no indeterminacy in the time evolution of a quantum system. Indeterminacy appears only when a physical quantity is measured.

> Between two measurements, the state vectors evolves (following Shcrodinger equation) in a perfectly deterministic way.

Supeorposition

The equation (1.8) is linear and homogeneous, then their slutions are linearly superposable:

$$|\psi(t_0)\rangle = \lambda_1|\psi_1(t_0)\rangle + \lambda_2|\psi_2(t_0)\rangle \Longrightarrow |\psi(t)\rangle = \lambda_1|\psi_1(t)\rangle + \lambda_2|\psi_2(t)\rangle. \tag{1.9}$$

Conservation of probability

Since the Hamiltonian operator $H(t)$ is Hermitian, the square of the norm of the state vector $\langle\psi(t)|\psi(t)\rangle$ does not depend on time:

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle &= \left[\frac{d}{dt}\langle\psi(t)|\right]|\psi(t)\rangle + \langle\psi(t)|\left[\frac{d}{dt}|\psi(t)\rangle\right] \\
&= \left[-\frac{1}{i\hbar}\langle\psi(t)|H(t)\right]|\psi(t)\rangle + \langle\psi(t)|\left[\frac{1}{i\hbar}H(t)|\psi(t)\rangle\right] \\
&= -\frac{1}{i\hbar}\langle\psi(t)|H(t)|\psi(t)\rangle + \frac{1}{i\hbar}\langle\psi(t)|H(t)|\psi(t)\rangle \\
\frac{d}{dt}\langle\psi(t)|\psi(t)\rangle &= 0.
\end{aligned}$$

The property of conservation of the norm which we have derived is expressed by the equation

$$\langle\psi(t)|\psi(t)\rangle = \int d^3r\ |\psi(\boldsymbol{r},t)|^2 = \langle\psi(t_0)|\psi(t_0)\rangle = 1. \tag{1.10}$$

This implies that time evolution does not modify the global probability of finding the particle in all space, which always remains equal to 1.

1.4.2 Conservative systems

When the Hamiltonian of a physical system **does not** depend explicitly on time, the system is said to be **conservative**. It can also be said that the total energy of the system is constant of the motion.

Solution of the Schrodinger equation

Lets consider the eigenequation of H (assuming discrete spectrum):

$$H|\varphi_{n,\tau}\rangle = E_n|\varphi_{n,\tau}\rangle. \tag{1.11}$$

τ is used to denote the set of indices other than n necessary to uniquely characterizes a unique vector $|\varphi_{n,\tau}\rangle$. Since H does not depend on time, neither E_n nor $|\varphi_{n,\tau}\rangle$. Because $|\varphi_{n,\tau}\rangle$ form a basis, it is always possible to expand the state $|\psi(t)\rangle$:

$$|\psi(t)\rangle = \sum_{n,\tau} c_{n,\tau}(t)|\varphi_{n,\tau}\rangle, \quad \text{with} \quad c_{n,\tau}(t) = \langle\varphi_{n,\tau}|\psi(t)\rangle.$$

All the time dependence of $|\psi(t)\rangle$ is contained within $c_{n,\tau}(t)$. Let us project the Schrodinger equation onto each of the states $|\varphi_{n,\tau}\rangle$:

$$i\hbar\frac{d}{dt}\langle\varphi_{n,\tau}|\psi(t)\rangle = \langle\varphi_{n,\tau}|H|\psi(t)\rangle$$
$$i\hbar\frac{d}{dt}c_{n,\tau}(t) = E_n c_{n,\tau}(t).$$

This equation can be integrated to give

$$c_{n,\tau}(t) = c_{n,\tau}(t_0)e^{-E_n(t-t_0)/\hbar}. \tag{1.12}$$

When H does not depend on time, to find $|\psi(t)\rangle$ given $|\psi(t_0)\rangle$, proceed as follows:

- Expand $|\psi(t_0)\rangle$ in terms of the eigenstates of H:

$$|\psi(t_0)\rangle = \sum_n \sum_\tau c_{n,\tau}(t_0)|\varphi_{n,\tau}\rangle, \quad \text{with} \quad c_{n,\tau}(t_0) = \langle\varphi_{n,\tau}|\psi(t_0)\rangle.$$

- To obtain $|\psi(t)\rangle$, multiply each coefficient $c_{n,\tau}(t_0)$ of the expansion by the term $e^{-iE_n(t-t_0)/\hbar}$:

$$|\psi(t)\rangle = \sum_n \sum_\tau c_{n,\tau}(t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle.$$

  or, in the continuous case,

$$|\psi(t)\rangle = \sum_\tau \int dE\; c_\tau(E, t_0)e^{-iE_n(t-t_0)/\hbar}|\varphi_{n,\tau}\rangle.$$

1.5 The superposition principle and physical predictions

One of the important consequences of the first postulate, when it is combined with the others, is the appearance of **interference effects**.

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