Lecture notes
MP462 Quantum Mechanics I
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1 Introduction

1.1 Origins of quantum

In this chapter, we will be interested in essential logical steps that led to quantum mechanics. We understand that quantum mechanics is a physical theory (the most complete we have), meaning it is a mathematically consistent theoretical construct which is able to explain and predict certain experimental observations which can not be explained within the framework of classical mechanics and classical (i.e. Maxwell) theory of electromagnetism. The specific focus of this section will be on development of the concept of wave-particle duality for both electromagnetic field and matter in the early times of quantum mechanics. We do not intend to present detailed or complete history of quantum theory which is beyond the scope of this course and can be found elsewhere and neither we present complete overview of unique features of quantum mechanics in this lecture as these will be subjects of the other lectures of this course.

Further reading: The early stages of the development of quantum mechanics with detailed discussion of relevant experiments is presented in *D. Bohm, Quantum Theory, 1951.* Also an excelent (and more historical) account of the same period (and particularly an important role played by Einstein) can be found in *A. Pais, Subtle is the Lord: The Science and the Life of Albert Einstein, 1983.*

1.1.1 Black-body radiation problem

A black-body is a body that absorbes all the electromagnetic radiation which falls on its surface. Rather than an ideally absorbing body, it can be physically realized as a hollow cavity in which electromagnetic radiation is trapped. The radiation is in thermal equilibrium with the surounding material, that is, with material oscillators of the cavity wall which continuously emit and absorb waves of any frequency. The higher is the temperature, the higher is the mean frequency of radiation inside the cavity.

The electromagnetic energy distribution inside the cavity as a function of frequency and temperature $U(\nu, T)$ is proportional to the intensity of the radiation per unit solid angle $I(\nu, T) = \frac{c}{4\pi} U(\nu, T)$. This can be measured through a small opening in the cavity (negligible compared to the area of the cavity surface) which allows the radiation to escape from the cavity without causing significant alteration of the radiation distribution inside. These measurents, which have been carried out since late 19th century (e.g. particularly noticeable experiments are those by Rubens and Kurlbaum (1900) due to their great precision and wide range of frequencies), revealed a single peak in the frequency dependence of the intensity $I(\nu, T)$. The experimental data however could not be entirely explained within the framework of classical physics. This discrepancy between experimental data and classical theoretical concepts constitutes what we know as the black-body radiation problem. Let us see first classical attempts by Wien (1896), Rayleigh and Jeans (1900) before going in more detail to quantum hypothesis by Planck (1900) which is historically considered the beginning of quantum theory.

In 1896, Wien used empirical data and thermodynamical arguments to explain the black-body radiation problem. He proposed the following distribution which is now known as the Wien law:

$$I(\nu, T) = a\nu^3 e^{-b\nu/k_B T} \tag{1}$$

where a and b are empirical constants, and k_B is the Boltzmann constant ($1.38 \times 10^{-23} JK^{-1}$).

Wien's law provided agreed very well with the experimental data for high frequencies, but clearly deviated from the experimental data at short frequencies where it showed lower intensity $I(\nu, T)$ than observed. Moreover, introduction of empirical constants (without really providing their physical interpretation) made this theory semiempirical.

In an atempt to explain new observations by Rubens and Kurlbaum in 1900, Rayleight used classical electromagnetism and theormodynamics to

derive the radiation distribution from the first principles. His work complemented by additional clarifications by Jeans resulted in the Rayleigh-Jeans law:

$$I(\nu, T) = \frac{2\nu^2}{c^2} k_B T \tag{2}$$

The formula well reproduces experimental observations at low frequencies but rapidly diverges at high frequencies. This behaviour, i.e.monotonic increase of radiation intensity with frequency, is known as ultraviolet catastrophe. Clearly this can not describe any realistic black-body radiation law.

The same year, Planck attacked the black-body problem by proposing quantum hypothesis, i.e. that the energy of electromagnetic radiation of a given frequency is emitted and absorbed in elementary packets called quanta, so the energy of the radiation of a given frequency ν is given as:

$$E_n = nh\nu \tag{3}$$

h is a new fundamental constant, known as the Planck constant (6.626×10^{-34}), and n is an integer. Planck then obtained the black-body radiation distribution now know as the Planck law in the following form:

$$I(\nu, T) = \frac{2h\nu^3}{c^2} \frac{e^{-h\nu/k_B T}}{1 - e^{-h\nu/k_B T}} \tag{4}$$

which perfectly reproduces experimental observations.

Outline of the Planck law derivation. The probability $W(n)$ that an classical oscillator has energy corresponding to its n-th harmonic (i.e. n-th value) is given as $W(n) \propto e^{-E/k_B T}$. Assuming that the same form holds also in the case of a quantum mechanical oscillator, whose energy is $E_n = nh\nu$, the probability is $W(n) \propto e^{-E_n/k_B T}$. The normalization of this probability, which ensures that $\sum_{n=0}^{\infty} W(n) = 1$, then lead to the equation

$$W(n) = \frac{e^{-nh\nu/k_B T}}{\sum_{n=0}^{\infty} e^{-nh\nu/k_B T}} = e^{-nh\nu/k_B T}(1 - e^{-h\nu/k_B T}) \tag{5}$$

To get the left hand side (i.e. $l.h.s.$) of the equation, we used the formula $\sum_{n=0}^{\infty} (e^{-x})^n = (1 - e^{-x})^{-1}$.

Now we can calculate the mean energy

$$< E >= \sum_{n=0}^{\infty} E_n W(n) = h\nu(1 - e^{-h\nu/k_B T}) \sum_{n=0}^{\infty} n e^{-nh\nu/k_B T} \tag{6}$$

which can be rewritten using the relation $\sum_{n=0}^{\infty} ne^{-nx} = -\frac{d}{dx}\sum_{n=0}^{\infty} e^{-nx} = -\frac{d}{dx}\frac{1}{1-e^{-x}} = \frac{e^{-x}}{(1-e^{-x})^2}$ as

$$< E >= \frac{h\nu e^{-h\nu/k_BT}}{1 - e^{-h\nu/k_BT}} \tag{7}$$

and multiplying this by the density of oscillators with the frequency ν , which is given as $\frac{8\pi}{c^3}\nu^2$, we get the energy distribution $U(\nu)$ and from that the desired intensity as given by Eq. (4).(Remark: derivation of the $U(\nu)$ is presented in *D. Bohm, Quantum Theory, 1951*; we may add this later to these notes, however it is not essential in the present context).

The classical results by Wien and by Rayleigh and Jeans agree with experimental data respectively at high and low frequencies. Hence, it must be possible to reconstruct both classical laws as appropriate limits of the Planck law. For small frequencies, i.e. $\frac{h\nu}{k_BT} << 1$, we can use the Taylor series to approximate $e^{-h\nu/k_BT}$ as $1 - \frac{-h\nu}{k_BT}$. Straightforward substitution of this relation into Eq.(4) gives the Rayleight-Jeans law $I(\nu, T) = \frac{2\nu^2}{c^2}k_BT$. In the opposite limit, i.e. $\frac{h\nu}{k_BT} >> 1$, the denominator in Eq.(4) can be approximated $1 - e^{-h\nu/k_BT} \sim 1$ and thus neglected. Eq.(4) then acquires the form of the Wien law $I(\nu, T) = \frac{2h\nu^3}{c^2}e^{-h\nu/k_BT}$. Note that the empirical constant a and b now got meaning.

1.2 Heat capacities problem

For a few years after its conception, the Planck quantization hypothesis lived only within the narrow field of black-body elelctromagnetic radiation. In 1906, Einstein extended it also to material systems and used it to resolved the problem of the specific heat capacities $C_V = \frac{\partial <E>}{\partial T}$ of solids. The relevant experimental observations showed that at high temperature the specific heat capacity C_V of solid materials converged to a plateau where $C_V = k_B$ while at low temperatures it converges to zero. To explain the temperature dependence of C_V, Einstein proposed that material oscilators (i.e. atoms bind in crystal structure) are quantized and, in contrast to electromagnetic waves which can have various frequencies, it permits only one frequency for all oscillators. The mean energy is given by Eq.(7) and the specific heat capacity is then expressed as

$$C_V = \frac{\partial < E >}{\partial T} = \frac{h^2\nu^2}{k_BT}\frac{e^{-h\nu/k_BT}}{(1 - e^{-h\nu/k_BT})^2} \tag{8}$$

The high temperature limit when $\frac{h\nu}{k_B T} \to 0$ then properly reproduces experimental observations giving $C_V = k_B$. The low temperature behaviour is given as $C_V = \frac{h^2\nu^2}{k_B T^2} e^{\frac{h\nu}{k_B T}}$. Precise measurements reveal that the experimental data obtained for realistic materials differ from theoretical low temperature behaviour; this is explained by mutual coupling of the material oscillators neglected in Einstein's approach.

1.3 Photoelectric effect

Photoelectric effect was first observed by Lennard (1902) and theoretically explained by Einstein (1905) be proposing that light consists of particles called photons. The photoelectric effect is the process where ultraviolet (UV) light which falls on a metalic surface ejects electrons with the kinetic energy $\frac{1}{2} m_e v^2$ from the metal. Here m_e and v are the electron mass and velocity respectively. Important is that the kinetic energy of outgoing electrons only depend on frequency of the incoming radiation but not on its intensity. Obviously, the electrons absorb the energy only in quanta, so that their kinetic energy is given as $\frac{1}{2} m_e v^2 = h\nu - W$ where W is a work function of the metal (it is a material constant which characterizes the binding energy of electron in the metal) and $h\nu$ is the energy of the UV light. In 1905, Einstein proposed that this experimental observations can be explain if we accept that the reason why the light energy is absorbed in quanta is that light consists of particles, photons, each carrying energy quantum $h\nu$.

1.4 Compton scattering

The Compton scattering, discovered experimentally by Compton (1922), is a process when an electromagnetic radiation with the initial momentum $\vec{p}_{in}$ scatters through a stationary electron. The momentum of the outgoing electron is $\vec{P}_{out}$. The electromagnetic radiation leaves the scattering event with the momentum $\vec{p}_{out}$ along the trajectory which is deflected from the original trajectory by an angle θ. The wavelength of the outgoing radiation is shifted compared to the incoming radiation as $\Delta\lambda = \lambda_{out} - \lambda_{in}$. This experiment is direct demonstration of the particle-like character of electromagnetic field.

1.5 de Broglie hypothesis

In 1923, de Broglie postulated particle-wave duality to material particles. In analogy to light which can be regarded as both electromagnetic waves and photons, every massive particle of the momentum $\vec{p}$ can be regarded as

a wave whose wavelength is given as

$$\lambda = \frac{h}{|\vec{p}|} \tag{9}$$

where $\vec{p} = m\vec{v}$ is a momentum. It is worth to note that this hypothesis was not based on any existing experimental observations but it rather predicted that the wave-like phenomena of material particles to be seen in future. This happened in experiments by Davisson and Germes in 1927, who observed difraction of electrons from a crystal. With the de Broglie hypothesis, the wave-particle duality becomes an essential property of every quantum mechanical system.

1.6 Other developments

Rutherford experiments (1911-1913) with scattering of α particles through atoms revealed that the most of the atomic mass is concentrated in the nuclei which is very small. This led to the idea of planetary model of atom in which electrons are orbiting around the positively charged nucleus along Kepler orbits. Clearly this idea was not sustainable on the ground of classical physics as orbiting electron would be loosing energy by irradiating electromagnetic waves and would eventually collaps to the nucleus, making atoms and thus matter quite unstable. The experiments by Franck and Hertz (1913) showed that spectral terms E_n/h are stable and definitive for each atom. Consequently Bohr postulated that a new model of atom in which electrons are orbiting only on fixed discrete trajectories. This represents an important step towards the quantum theory of atoms and molecules which we will encounter towards the end of the course.

Other important developments include formulation of matrix mechanics (1925), and also development of Schroedinger wave mechanics (1926). It has been shown later that both approaches are equivalent. We will be discussing these within the other lectures of this course along with other strange features of quantum mechanics including e.g. uncertainty relations, entanglement, measurement problem etc.

2 Mathematical foundations

A state of a physical system is represented by a vector in the Hilbert space.

Composition of Hilbert spaces Let $\mathcal{H}_1$ be a subspace of the Hilbert space $\mathcal{H}$. For $\forall|\,\psi\rangle$ orthogonal to all the vectors in $\mathcal{H}_1$ form a vector space $\mathcal{H}_1^{\perp}$ (an orthogonal complement $\mathcal{H}_1$) .

Let $\mathcal{H}_1, \mathcal{H}_2, ..., \mathcal{H}_n$ be subspaces of $\mathcal{H}$ (n can be infinite). An element of $\mathcal{H}_1$ can be written as a linear combination of vectors from $\mathcal{H}_1, \mathcal{H}_2, ..., \mathcal{H}_n$ for all $i \neq k = 1, 2, ..., n$ and for all $|\,\psi_i\rangle \in \mathcal{H}_i$ and $|\,\psi_k\rangle \in \mathcal{H}_k$ such that $\langle\psi_i|\psi_k\rangle = 0$, we say that $\mathcal{H}$ is a direct sum of (mutually orthogonal) subspaces $\mathcal{H}_1, \mathcal{H}_2, ..., \mathcal{H}_n$

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus ... \oplus \mathcal{H}_n = \bigoplus_{j=1}^{k=n} \mathcal{H}_k \tag{10}$$

Important role in quantum mechanics is played by tensor product of Hilbert spaces. Consider $\mathcal{H}_1$ and $\mathcal{H}_2$ of the dimension as N_1 and N_2 respectively. Let $|\,\psi_n^{(j)}\rangle$, $n = 1, 2, ..., N$ and $j = 1, 2$, form a basis of $\mathcal{H}_j$. The vectors $|\,\psi_n^{(1)}\rangle|\,\psi_m^{(2)}\rangle$ can be identified with elements of the orthonormal basis of the Hilbert space $\mathcal{H}$, with the dimension $dim(\mathcal{H}) = N_1 \times N_2$

$$|\,\phi\rangle = |\,\psi_n^{(1)}\rangle|\,\psi_m^{(2)}\rangle \tag{11}$$

where $j = (n-1)N_2 + m$. The scalar product is defined as

$$\langle\phi_j|\phi_{j'}\rangle = \langle\psi_n^{(1)}|\psi_{n'}^{(1)}\rangle\langle\psi_n^{(2)}|\psi_{n'}^{(2)}\rangle = \delta_{nn'}\delta_{mm'} = \delta_{jj'} \tag{12}$$

We say that $\mathcal{H}$ is a tensor product of $\mathcal{H}_1$ and $\mathcal{H}_2$, $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$.

For $\forall\phi \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$) can be written as

$$|\,\phi\rangle = \sum_{j=1}^{N} a_j|\,\phi_j\rangle = \sum_{n=1}^{N_1}\sum_{m=1}^{N_2} = a_{nm}|\,\psi_n^{(1)}\rangle|\,\psi_m^{(2)}\rangle \tag{13}$$

and if $a_{nm} = \alpha_n\beta_m$, then $|\,\phi\rangle = |\,A\rangle|\,B\rangle$ where $|\,A\rangle = \sum_{n=1}^{N_1}\alpha_n|\,\psi_n^{(1)}\rangle \in \mathcal{H}$ and $|\,B\rangle = \sum_{m=1}^{N_2}\beta_n|\,\psi_n^{(2)}\rangle \in \mathcal{H}$. we say that $ket\phi$ is a direct product of the vectors $|\,A\rangle$ and $|\,B\rangle$.

We can define concepts analogous for real functions also for vector functions. Let $\xi \in \mathbb{C}$, a complex vector function is a map $\xi \to |\,\psi(\xi)\rangle$ where $|\,\psi(\xi)\rangle$ is a vector. For example we can define a derivative through the concept of limit as done in mathematical analysis. We can use this to define derivative of an inner product

$$\frac{d}{d\xi}\langle\phi(\xi)|\psi(\xi)\rangle = (\frac{d}{d\xi}\langle\phi(\xi)\,|)|\,\psi(\xi)\rangle + \langle\phi(\xi)\,|(\frac{d}{d\xi}|\,\psi(\xi)\rangle) \tag{14}$$

where the first term of r.h.s. corresponds to the bra vector of the ket $\frac{d}{d\xi}|\,\phi(\xi)\rangle$.

Examples of Hilbert spaces

1. U^n space is n-dimensional Hilbert space formed by all $(1 \times n)$-matrices whose entries are complex numbers

$$|\,\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ ... \\ a_n \end{pmatrix} \tag{15}$$

where multiplication by a complex scalar and sum are carried out in a usual way. The inner product is defined as

$$\hat{A} = \begin{pmatrix} a_1^* a_2^* ... a_n^* \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ ... \\ a_n \end{pmatrix} = \sum_{j=1}^{n} a_j^* b_j \tag{16}$$

2. Space l^2 is an infinite dimensional vector space of $(1 \times \infty)$-matrices such that $\sum_{j=1}^{\infty} |a_j|^2 < \infty$.

3. Space $L^2(a, b)$ is formed by all complex functions $A(\xi)$ of a real variable ξ that are square integrable (in the sense of the Lebesgue integral), i.e.

$$\int_a^b |A(\xi)|^2 d\xi < \infty \tag{17}$$

The scalar product is defined as follows

$$\langle A|B\rangle = \int_a^b A(\xi)^* B(\xi) d\xi \tag{18}$$

2.1 Operator theory

Definition. An operator $\hat{A}$ between the Hilbert spaces $\mathcal{U}$ and $\mathcal{V}$ is a function which to every vector $|\,\psi\rangle \in \mathcal{U}$ assigns a vector $|\,\psi\rangle' \in \mathcal{V}$. We write

$$|\,\psi\rangle' = \hat{A}|\,\psi\rangle \tag{19}$$

$\hat{U}$ is called the domain of the operator $\hat{A}$, $D(\hat{A})$. The set $R(\hat{A}) = \{|\,\psi\rangle' = \hat{A}|\,\psi\rangle | \forall |\,\psi\rangle \in \mathcal{U}\}$ is called the range of the operator $\hat{A}$.

Examples. We list several simple examples of operators:

1. The operator $\hat{A}_1 = \lambda \in \mathbb{C}$ acts on a vector $|\,\psi\rangle$ as $\hat{A}_1|\,\psi\rangle = \lambda|\,\psi\rangle$.

   Note that if $\lambda = 1$, this operator acts as the identity operator $\hat{1}$: $\hat{1}|\,\psi\rangle = |\,\psi\rangle$.

2. $\hat{A}_2|\,\psi\rangle = \frac{1}{\sqrt{\langle\psi|\psi\rangle}}|\,\psi\rangle$ normalizes a vector $|\,\psi\rangle$.

3. $\hat{A}_3|\,\psi\rangle = \langle\psi|\psi\rangle|\,\psi\rangle$ multiplies a vector $|\,\psi\rangle$ by the square of its norm.

4. $\hat{A}_4 = |\,\phi\rangle\langle\phi\,|$ acts as $\hat{A}_4|\,\psi\rangle = \langle\phi|\psi\rangle|\,\phi\rangle$.

   The operators $\hat{A}_4$ and $\hat{A}_3$ look similar but there is actually a fundamental difference between them. We can see this if we apply them on a quantum state $|\,\psi\rangle = c_1|\,\psi_1\rangle + c_2|\,\psi_2\rangle$:

   $$\hat{A}_4|\,\psi\rangle = \hat{A}_4(c_1|\,\psi_1\rangle + c_2|\,\psi_2\rangle) = c_1\hat{A}_4|\,\psi_1\rangle + c_2\hat{A}_4|\,\psi_2\rangle \tag{20}$$

   here we say that the operator $\hat{A}_4$ is linear. However no such relation holds for $\hat{A}_3$ as we can see from the following

   $$\begin{aligned}&\hat{A}_3|\,\psi\rangle = \langle\psi|\psi\rangle|\,\psi\rangle = \\ &(|c_1|^2\langle\psi_1|\psi_1\rangle + c_1^*c_2\langle\psi_1|\psi_2\rangle + c_1c_2^*\langle\psi_2|\psi_1\rangle + |c_2|^2\langle\psi_2|\psi_2\rangle)|\,\psi\rangle \neq \\ &c_1\hat{A}_3|\,\psi_1\rangle + c_2\hat{A}_3|\,\psi_2\rangle = c_1\langle\psi_1|\psi_1\rangle|\,\psi_1\rangle + c_2\langle\psi_2|\psi_2\rangle|\,\psi_2\rangle\end{aligned} \tag{21}$$

Linearity and basic algebraic properties of operators. Linearity of operators is a very important property as operators relevant to quantum mechanics are linear operators. We say that an operator $\hat{A}$ is linear iff it satisfies

$$\hat{A}\sum_i c_i|\,\psi\rangle = \sum_i c_i\hat{A}|\,\psi\rangle \tag{22}$$

In this sense, quantum mechanics is a linear theory.

Let $\hat{A}, \hat{B}$ and $\hat{C}$ be linear operators. We say that

1. $\hat{A}$ and $\hat{B}$ are equal, $\hat{A} = \hat{B}$, if

$$\begin{aligned} \hat{A}|\,\psi\rangle &= \hat{B}|\,\psi\rangle \\ D(\hat{A}) &= D(\hat{B}). \end{aligned} \tag{23}$$

   for $\forall|\,\psi\rangle$.

2. $\hat{C}$ is a sum of $\hat{A}$ and $\hat{B}$, $\hat{C} = \hat{A} + \hat{B}$, if

$$\hat{C}|\,\psi\rangle = \hat{A}|\,\psi\rangle + \hat{B}|\,\psi\rangle. \tag{24}$$

   for $\forall|\,\psi\rangle$.

3. $\hat{C}$ is a product of $\hat{A}$ and $\hat{B}$, $\hat{C} = \hat{A}\hat{B}$,

$$\hat{C}|\,\psi\rangle = \hat{A}\hat{B}|\,\psi\rangle = \hat{A}(\hat{B}|\,\psi\rangle) = \hat{A}|\,\hat{B}\psi\rangle. \tag{25}$$

   for $\forall|\,\psi\rangle$.

Specifically, note that $\hat{A}^2 = \hat{A}\hat{A}$ and analogously $\hat{A}^n = \hat{A}\hat{A}^{n-1}$. If a function f can be expanded in a power series

$$f(\xi) = \sum_n a_n \xi^n \tag{26}$$

where ξ is a variable, then by the function of an operator $f(\hat{A})$ we mean

$$f(\hat{A}) = \sum_n a_n \hat{A}^n \tag{27}$$

A very useful example is an exponential function

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n \tag{28}$$

Commutator and anti-commutator. In contrast to numbers, real or complex, a product of operators is generally not commutative which means that $\hat{A}\hat{B} \neq \hat{B}\hat{A}$.

For example, let us have three vectors $|\,x\rangle$, $|\,y\rangle$, and $|\,z\rangle$, and the operators $\hat{R}_x$ and $\hat{R}_y$ such that

$$\begin{aligned} \hat{R}_x|\,x\rangle &= |\,x\rangle \\ \hat{R}_x|\,y\rangle &= |\,z\rangle \\ \hat{R}_x|\,z\rangle &= -|\,y\rangle \\ \hat{R}_y|\,x\rangle &= -|\,z\rangle \\ \hat{R}_y|\,y\rangle &= |\,y\rangle \\ \hat{R}_y|\,z\rangle &= |\,x\rangle \end{aligned} \tag{29}$$

then

$$\hat{R}_x\hat{R}_y|\,z\rangle = \hat{R}_x|\,x\rangle = |\,x\rangle \neq \hat{R}_y\hat{R}_x|\,z\rangle = -\hat{R}_y|\,y\rangle = -|\,y\rangle \tag{30}$$

An operator $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is called commutator of the operators $\hat{A}$ and $\hat{B}$. If $[\hat{A},\hat{B}] = 0$, we say that $\hat{A}$ and $\hat{B}$ commute. If $[\hat{A},\hat{B}] = 0$ then also $[f(\hat{A}), f(\hat{B})] = 0$.

An operator $\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is called anticommutator of the operators $\hat{A}$ and $\hat{B}$. If $\{\hat{A},\hat{B}\} = 0$, we say that $\hat{A}$ and $\hat{B}$ anticommute.

Basic properties of commutators and anticommutators are summarized below:

$$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}] \tag{31}$$
$$[\hat{A},\hat{B}+\hat{C}] = [\hat{A},\hat{B}] + [\hat{A},\hat{C}] \tag{32}$$
$$[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}] = \{\hat{A},\hat{B}\}\hat{C} - \hat{B}\{\hat{A},\hat{C}\} \tag{33}$$
$$[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B} = \hat{A}\{\hat{B},\hat{C}\} - \{\hat{A},\hat{C}\}\hat{B} \tag{34}$$

$$\{\hat{A},\hat{B}\} = \{\hat{B},\hat{A}\} \tag{35}$$
$$\{\hat{A},\hat{B}\hat{C}\} = \{\hat{A},\hat{B}\}\hat{C} - \hat{B}[\hat{A},\hat{C}] = \hat{B}\{\hat{C},\hat{A}\} - [\hat{B},\hat{A}]\hat{C} \tag{36}$$
$$\{\hat{A}\hat{B},\hat{C}\} = \hat{A}\{\hat{B},\hat{C}\} - [\hat{A},\hat{C}]\hat{B} = \{\hat{C},\hat{A}\}\hat{B} - \hat{A}[\hat{B},\hat{C}] \tag{37}$$

Another important property is given by the Jacobi identity:

$$[\hat{A}[\hat{B},\hat{C}]] + [\hat{B}[\hat{C},\hat{A}]] + [\hat{C}[\hat{A},\hat{B}]] = 0 \tag{38}$$

Classes of operators An operator $\hat{A}$ is called bounded iff $\exists\beta > 0$ such that:

$$\|\hat{A}|\,\psi\rangle\| \leq \beta\||\,\psi\rangle\| \tag{39}$$

for $\forall|\,\psi\rangle \in D(\hat{A})$. The symbol $\|.\|$ means the norm. The infimum of β is called the norm of an operator. In finite dimensional Hilbert spaces, all operators are bounded. Sum and product of bounded operators is a bounded operator because

$$\begin{aligned}\|\hat{A}+\hat{B}\| &\leq \|\hat{A}\| + \|\hat{B}\| \\ \|\hat{A}\hat{B}\| &\leq \|\hat{A}\|\|\hat{B}\|\end{aligned} \tag{40}$$

Specially

$$\|\lambda\hat{A}\| = |\lambda|\|\hat{A}\| \tag{41}$$

An operator $\hat{A}$ is called symmetric if

$$\langle\psi_1|\hat{A}\psi_2\rangle = \langle\hat{A}\psi_1|\psi_2\rangle \tag{42}$$

for $\forall|\,\psi_1\rangle, |\,\psi_2\rangle \in D(\hat{A})$ (dense in the Hilbert space $\mathcal{H}$).

An operator $\hat{A}$ is called hermitian if it is bounded and symmetric. It is called antihermitian if the operator $i\hat{A}$ is hermitian.

Let $\hat{A}$ be a bounded operator with the domain dense in the Hilbert space $\mathcal{H}$, then there is an adjoint operator $\hat{A}^\dagger$ such that

$$\langle\psi_1|\hat{A}^\dagger\psi_2\rangle = \langle\hat{A}\psi_1|\psi_2\rangle \tag{43}$$

that is

$$\langle\psi_1|\hat{A}^\dagger\psi_2\rangle = \langle\psi_2|\hat{A}\psi_1\rangle^* \tag{44}$$

for $\forall|\,\psi_1\rangle, |\,\psi_2\rangle \in D(\hat{A})$.

The following identities hold

$$\begin{aligned}
\|\hat{A}^\dagger\| &= \|\hat{A}\| && (45)\\
(\hat{A}^\dagger)^\dagger &= \hat{A} && (46)\\
(\hat{A}+\hat{B})^\dagger &= \hat{A}^\dagger + \hat{B}^\dagger && (47)\\
(\hat{A}\hat{B})^\dagger &= \hat{B}^\dagger\hat{A}^\dagger && (48)\\
(\lambda\hat{A})^\dagger &= \lambda^*\hat{A}^\dagger && (49)
\end{aligned}$$

and, for some fixed vectors $|\,\phi_1\rangle$ and $|\,\phi_2\rangle$ we can define an operator $\hat{A}_{j,k} = |\,\phi_j\rangle\langle\phi_k\,|$ (where $j,k \in \{1,2\}$) then

$$\hat{A}^\dagger_{j,k} = \hat{A}_{k,j} \tag{50}$$

An operator $\hat{A}$ is self-adjoint if

$$\hat{A}^\dagger = \hat{A} \tag{51}$$

These operators are particularly important in quantum mechanics as they represent observable physical quantities; hence we call these operators observables. As we will see later, they possess real spectrum, i.e. their eigenvalues are real numbers $\mathbb{R}$.

An operator $\hat{A}$ is positive if $\langle\psi\,|\hat{A}|\,\psi\rangle \geq 0 \text{for} \forall|\,\psi\rangle$.

An operator $\hat{A}$ is normal if $[\hat{A}, \hat{A}^\dagger] = 0$.

Let $\hat{A}$ be an operator. If there exist an operator $\hat{A}^{-1}$ such that $\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \hat{1}$, then it is called an inverse operator to $\hat{A}$. The following properties hold

$$\begin{aligned}
(\hat{A}\hat{B})^{-1} &= \hat{B}^{-1}\hat{A}^{-1} && (52)\\
(\hat{A}^\dagger)^{-1} &= (\hat{A}^{-1})^\dagger. && (53)
\end{aligned}$$

Remark: in finite dimensional space $\hat{A}\hat{B} = 1$ implies $\hat{B}\hat{A} = 1$ but this is generally not true in the infinite dimensional spaces and that is why we need both $\hat{A}\hat{A}^{-1}$ and $\hat{A}^{-1}\hat{A}$ above.

An operator $\hat{U}$ is called unitary if $\hat{U}^\dagger = \hat{U}^{-1}$ and $D(\hat{U}) = \mathcal{H}$. This is a very important class of operators as they are formal solution of the Schödinger equation and thus represent quantum dynamics. Also important groups of symmetries are unitary.

The unitary operators are isometric $\langle \hat{U}\psi_1 | \hat{U}\psi_2 \rangle = \langle \psi_1 | \psi_2 \rangle$.Also, let the set $\{ | \psi_i \rangle \}$ is a basis of the Hilbert space $\mathcal{H}$ and $\hat{U}$ is a unitary operator, then $\{ \hat{U} | \psi_i \rangle \}$ is also a basis of $\mathcal{H}$.

The fundamental theorem by Wigner significantly restricts what operators can represent symmetry operation on the Hilbert space of physical states. Consider maps of $\mathcal{H}$ onto itself $| \psi \rangle \to | \psi' \rangle$ such that $|\langle \psi_1 | \psi_2 \rangle = \langle \psi_1' | \psi_2' \rangle, \forall | \psi_{1,2} \rangle \in \mathcal{H}$, then $| \psi' \rangle = e^{i\omega(\psi)} \hat{U} | \psi \rangle$ where $\hat{U}$ is a unitary operator which is either linear or antilinear and $\omega(\psi) \in \mathbb{R}$ is a phase that may depend on $| \psi \rangle$.

A bounded operator $\hat{P}$ satisfying

$$\hat{P} = \hat{P}^\dagger = \hat{P}^2 \tag{54}$$

is called a projection operator or simply projector. This class of operators is very important in quantum mechanics, particularly in the context of quantum measurement.

Let $\hat{P}_1$ be a projector, then $\hat{P}_2 = \hat{1} - \hat{P}_1$ is also a projector, with the following properties:

$$\hat{P}_1 + \hat{P}_2 = \hat{1} \tag{55}$$

$$\hat{P}_1 \hat{P}_2 = 0 \tag{56}$$

where the earlier is called the completeness relation (se below) and the latter expresses orthogonality.

For every vector $| \psi \rangle \in \mathcal{H}$ the following holds

$$| \psi \rangle = | \psi_1 \rangle + | \psi_2 \rangle$$

$$\langle \psi_1 | \psi_2 \rangle = 0$$

$$| \psi_1 \rangle = \hat{P}_1 | \psi \rangle \tag{57}$$

$$| \psi_2 \rangle = \hat{P}_2 | \psi \rangle \tag{58}$$

All vectors $| \psi_j \rangle, (j = 1, 2)$ for a subspace $\mathcal{H}_j \subset \mathcal{H}$, that is the projectors $\hat{P}_1$ and $\hat{P}_2$ assign to each vector from $\mathcal{H}$ its projection onto the subspace $\mathcal{H}_1$

and $\mathcal{H}_2$ respectively. These projections are mutually orthogonal as can be see from the relations above.

If the projector operators $\hat{P}_1$ and $\hat{P}_2$ satisfy $\hat{P}_1\hat{P}_2 = \hat{P}_1$ then the corresponding subspaces satisfy $\mathcal{H}_1 \subset \mathcal{H}_2$; we then say $\hat{P}_1 \leq \hat{P}_2$.

Let $|\,\psi_k\rangle$ be a normalized vector, then the operator

$$\hat{P}_k = |\,\psi_k\rangle\langle\psi_k\,| \tag{59}$$

is projection onto one-dimensional space spanned by all vectors linearly dependent on $|\,\psi_k\rangle$.

If vectors $\{|\,\psi_k\rangle\}$ form a basis of $\mathcal{H}_1$ then

$$\sum_k \hat{P}_k = \sum_k |\,\psi_k\rangle\langle\psi_k\,| \tag{60}$$

is projection operator onto $\mathcal{H}_1$. Furthermore if $\mathcal{H}_1 = \mathcal{H}$ then this projection is an identity operator

$$\sum_k |\,\psi_k\rangle\langle\psi_k\,| = \hat{1} \tag{61}$$

This relation known as the completeness relation has a prominent role in quantum mechanics.

Composition of operators Let $\mathcal{H}_1 \subset \mathcal{H}$. We say that $\mathcal{H}_1$ is invariant with respect to an operator $\hat{A}$ if $\forall|\,\psi_1\rangle \in \mathcal{H}_1$, $\hat{A}|\,\psi_1\rangle \in \mathcal{H}_1$.

We say that $\mathcal{H}_1$ reduces $\hat{A}$ if the subspace $\mathcal{H}_1$ and its orthogonal complement $\mathcal{H}_1^{\perp}$ are invariant with respect to $\hat{A}$.

Let $\mathcal{H}_i$, $i = 1, 2, ..., k$, reduce the operator $\hat{A}$. Let us define operators $\hat{A}_i$ with domain $D(\hat{A}_i) = \mathcal{H}_i$ such that $\forall|\,\psi_i\rangle \in \mathcal{H}_i$, $\hat{A}_i|\,\psi_i\rangle = \hat{A}|\,\psi_i\rangle$. Then

$$\hat{A}|\,\psi_i\rangle = \sum_{i=1}^{k} \hat{A}_i|\,\psi_i\rangle \tag{62}$$

We say that $\hat{A}$ is a direct sum of the operators $\hat{A}_i$

$$\hat{A} = \hat{A}_1 \oplus \hat{A}_2 \oplus ... \oplus \hat{A}_k = \bigoplus_{i=1}^{k} \hat{A}_i \tag{63}$$

Example: An operator $\hat{A}$ in the Hilbert space $\mathcal{U}^5$

$$\hat{A} = \begin{pmatrix} a_{11} & a_{12} & 0 & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} & a_{35} \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & a_{53} & a_{54} & a_{55} \end{pmatrix} \tag{64}$$

is the direct sum $\hat{A} = \hat{A}_1 \oplus \hat{A}_2$ of the operators $\hat{A}_1$ and $\hat{A}_2$

$$\hat{A}_1 = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \tag{65}$$

$$\hat{A}_2 = \begin{pmatrix} a_{33} & a_{34} & a_{35} \\ a_{43} & a_{44} & a_{45} \\ a_{53} & a_{54} & a_{55} \end{pmatrix} \tag{66}$$

where $\hat{A}_1$ and $\hat{A}_2$ act in the Hilbert spaces $\mathcal{U}^2$ and $\mathcal{U}^3$ respectively.

The following properties of the direct sum are important

$$Tr(\hat{A}_1 \oplus \hat{A}_2) = Tr\hat{A}_1 + Tr\hat{A}_2 \tag{67}$$

$$det(\hat{A}_1 \oplus \hat{A}_2) = det\hat{A}_1 . det\hat{A}_2 \tag{68}$$

If $\hat{A} = \hat{A}_1 \oplus \hat{A}_2$ and $\hat{B} = \hat{B}_1 \oplus \hat{B}_2$, and $\hat{A}_1$ and $\hat{B}_1$ act in the same Hilbert space, and so does $\hat{A}_2$ and $\hat{B}_2$, then $\hat{A}\hat{B} = \hat{A}_1\hat{B}_1 \oplus \hat{A}_2\hat{B}_2$.

A particularly important in the context of quantum mechanics is the direct product of operators which describes the composition of operators acting on distinct subsystems of a quantum mechanical system. Let $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, and $\hat{A}_j$, $j = 1, 2$ is an operator in $\mathcal{H}_j$ with the domain $D(\hat{A}_j)$. An operator $\hat{A} = \hat{A}_1 \otimes \hat{A}_2$ in $\mathcal{H}$ is a direct product of $\hat{A}_1$ and $\hat{A}_2$ and is defined as

$$\hat{A}|\,\psi_1\rangle|\,\psi_2\rangle = |\,\hat{A}_1\psi_1\rangle|\,\hat{A}_2\psi_2\rangle \tag{69}$$

for $\forall|\,\psi_j\rangle \in D(\hat{A}_j)$, and its domain is $D(\hat{A}) = D(\hat{A}_1)D(\hat{A}_2)$.

A useful example of a direct product of operators can be again given within the finite dimensional case. Let us have the operators

$$\hat{B} = \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix} \tag{70}$$

$$\hat{C} = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \tag{71}$$

the direct product is then constructed as

$$\hat{A} = \hat{B} \otimes \hat{C} = \begin{pmatrix} b_{11}c_{11} & b_{11}c_{12} & b_{12}c_{11} & b_{12}c_{12} & b_{13}c_{11} & b_{13}c_{12} \\ b_{11}c_{21} & b_{11}c_{22} & b_{12}c_{21} & b_{12}c_{22} & b_{13}c_{21} & b_{13}c_{22} \\ b_{21}c_{11} & b_{21}c_{12} & b_{22}c_{11} & b_{22}c_{12} & b_{23}c_{11} & b_{23}c_{12} \\ b_{21}c_{21} & b_{21}c_{22} & b_{22}c_{21} & b_{22}c_{22} & b_{23}c_{21} & b_{23}c_{22} \\ b_{31}c_{11} & b_{31}c_{12} & b_{32}c_{11} & b_{32}c_{12} & b_{33}c_{11} & b_{33}c_{12} \\ b_{31}c_{21} & b_{31}c_{22} & b_{32}c_{21} & b_{32}c_{22} & b_{33}c_{21} & b_{33}c_{22} \end{pmatrix} \tag{72}$$

We of course notice that

$$\hat{A} = \hat{B} \otimes \hat{C} = \begin{pmatrix} b_{11}\hat{C} & b_{12}\hat{C} & b_{13}\hat{C} \\ b_{21}\hat{C} & b_{22}\hat{C} & b_{23}\hat{C} \\ b_{31}\hat{C} & b_{32}\hat{C} & b_{33}\hat{C} \end{pmatrix} \tag{73}$$

Eigenvalues and eigenvectors. Let $|\,\psi_\alpha\rangle$ be a nonzero vector such that

$$\hat{A}|\,\psi_\alpha\rangle = \alpha|\,\psi_\alpha\rangle \tag{74}$$

then α is called an eigenvalue of $\hat{A}$ and $|\,\psi_\alpha\rangle$ is called an eigenvector of $\hat{A}$ corresponding to the eigenvalue α. If there is $n > 1$ vectors satisfying this equation for α we then say that eigenvalue α is n-fold degenerate.

The eigenvalues of a self-adjoint operator $\hat{A}$, which represent physical quantities in quantum mechanics, are real numbers:

$$\alpha\langle\psi_\alpha|\psi_\alpha\rangle = \langle\psi_\alpha|\hat{A}\psi_\alpha\rangle = \langle\hat{A}\psi_\alpha|\psi_\alpha\rangle^* = \alpha^*\langle\psi_\alpha|\psi_\alpha\rangle \tag{75}$$

and thus $\alpha = \alpha^*$ which is indeed possible only for real numbers.

Eigenvectors of self-adjoint operators corresponding to distinct eigenvalues are orthogonal. If $\beta \neq \alpha$ is also an eigenvalue of $\hat{A}$ then $\langle\psi_\alpha|\hat{A}\psi_\beta\rangle = \beta\langle\psi_\alpha|\psi_\beta\rangle$ and also

$$\langle\psi_\alpha|\hat{A}\psi_\beta\rangle = \langle\psi_\beta|\hat{A}\psi_\alpha\rangle^* = \alpha\langle\psi_\beta|\psi_\alpha\rangle^* = \alpha\langle\psi_\alpha|\psi_\beta\rangle \tag{76}$$

which implies that $\langle\psi_\alpha|\psi_\beta\rangle = 0$.

Operator is uniquely defined from its action on the basis vectors of the Hilbert space. Let $\mathcal{B} = \{|\,\psi_j\rangle\}$ is a basis of $\mathcal{H}(= D(\hat{A}))$,

$$\hat{A}|\,\psi_j\rangle = \sum_k |\,\psi_k\rangle\langle\psi_k\,|\hat{A}|\,\psi_j\rangle = \sum_k A_{kj}|\,\psi_k\rangle \tag{77}$$

where $A_{kj} = \langle\psi_k\,|\hat{A}|\,\psi_j\rangle$ are the matrix elements of the operator $\hat{A}$ in the matrix representation given by the basis $\mathcal{B}$.

For practical calculations we write the operator $\hat{A}$ as

$$\hat{A} = \sum_{kj} |\,\psi_k\rangle\langle\psi_k\,|\hat{A}|\,\psi_j\rangle\langle\psi_j\,| = \sum_{kj} A_{kj}|\,\psi_k\rangle\langle\psi_j\,| \tag{78}$$

We can now define an operator by its eigenrepresentation. Assume that the eigenvectors of $\hat{A}$ define a basis of the Hilbert space, $\mathcal{B} = \{|\,\psi_j\rangle\}$, then $A_{kj} = \langle\psi_k\,|\hat{A}|\,\psi_j\rangle = \alpha_j\delta_{kj}$. Operator in its eigenrepresentation is a diagonal matrix with eigenvalues on the diagonal

$$\hat{A} = \sum_{kj} |\,\psi_k\rangle\langle\psi_k\,|\hat{A}|\,\psi_j\rangle\langle\psi_j\,| = \sum_{kj} A_{kj}|\,\psi_k\rangle\langle\psi_j\,| \tag{79}$$

$$= \sum_{j} \alpha_j|\,\psi_j\rangle\langle\psi_j\,| = \sum_{j} \alpha_j\hat{E}_j \tag{80}$$

where $\hat{E}_j$ is a projector to a one-dimensional space defined by $|\,\psi_j\rangle$. We call the last expression also a spectral decomposition of the operator $\hat{A}$.

Process of obtaining eigenvalues and eigenvectors of operators is the most important part of solving quantum mechanical systems. Let A be a matrix representation of the operator $\hat{A}$. To find the eigenvalues (and eigenvectors), we are looking for unitary matrix U that would transform the matrix A into its diagonal form D, $D = U^\dagger AU$. Two operators commute iff there exist a unitary transformation which diagonalizes them simultaneously.

In practice, to get the eigenvalues, we have to solve the characteristic (or secular) equation defined as

$$det(A - \lambda\mathbf{1}) = \mathbf{0} \tag{81}$$

where $\mathbf{1}$ is the identity matrix.

Given a spectral decomposition of an operator $\hat{A} = \sum_j \alpha_j\hat{E}_j$. A function of the operator $\hat{A}$ can be defined as $f(\hat{A}) = \sum_j f(\alpha_j)\hat{E}_j$. Specially if $f = 1$ we get the completeness relation $1 = \sum_j \hat{E}_j$.

Complete set of observables. Let $\hat{A}^{(1)}, \hat{A}^{(2)}, ..., \hat{A}^{(M)}$ be a set of mutually commuting operators. We say that these operators form a complete set of commuting operators if each of the nonzero operators

$$\hat{I}^{(12...M)}_{j_1 j_2 ... j_M} = \hat{I}^{(1)}_{j_1}\hat{I}^{(2)}_{j_2}...\hat{I}^{(M)}_{j_M} \tag{82}$$

project to ne-dimensional subspace, i.e. for each M-tuple of eigenvalues $\alpha^{(1)}_{j_1}\alpha^{(2)}_{j_2}...\alpha^{(M)}_{j_M}$, there is maximally one linearly independent vector

$$|\,\alpha^{(1)}_{j_1}, \alpha^{(2)}_{j_2}, ..., \alpha^{(M)}_{j_M}\rangle \tag{83}$$

satisfying

$$\hat{A}^{(k)}|\,\alpha_{j_1}^{(1)},\alpha_{j_2}^{(2)},...,\alpha_{j_M}^{(M)}\rangle=\alpha_{j_k}^{(k)}|\,\alpha_{j_1}^{(1)},\alpha_{j_2}^{(2)},...,\alpha_{j_M}^{(M)}\rangle \tag{84}$$

where $k=1,...,M$ and $\|\,|\,\alpha_{j_1}^{(1)},\alpha_{j_2}^{(2)},...,\alpha_{j_M}^{(M)}\rangle\,\|=1$. In this case the projectors are explicitly

$$\hat{I}_{j_1j_2...j_M}^{(12...M)}=|\,\alpha_{j_1}^{(1)},\alpha_{j_2}^{(2)},...,\alpha_{j_M}^{(M)}\rangle\langle\alpha_{j_1}^{(1)},\alpha_{j_2}^{(2)},...,\alpha_{j_M}^{(M)}\,| \tag{85}$$

Mutually commuting operators $\hat{A}^{(1)},\hat{A}^{(2)},...,\hat{A}^{(M)}$ form a complete set of commuting operators iff an arbitrary operator commuting with all $\hat{A}^{(k)}$, $k=1,...,M$ is a function of the operators $\hat{A}^{(1)},\hat{A}^{(2)},...,\hat{A}^{(M)}$.

Generalization to the continuous spectrum Let $\hat{A}$ is an arbitrary operator with a continuous spectrum $\hat{A}|\,\alpha\rangle=\alpha|\,\alpha\rangle$. The normalization is given as $\langle\alpha|\alpha'\rangle=\delta(\alpha-\alpha')$ where $\delta(\alpha-\alpha')$ which we can understand as a generalization of the Kronecker delat for the continuous case (more details about the delta function as presented at lectures can be found in C. Cohen-Tannoudji, Quantum Mechanics II, the Appendix II).

The spectral decomposition in the continuous case is defined as

$$\hat{A}=\int_{\alpha_{min}}^{\alpha_{max}}\alpha|\,\alpha\rangle\langle\alpha\,|d\alpha \tag{86}$$

and the completeness relation is

$$\int_{\alpha_{min}}^{\alpha_{max}}|\,\alpha\rangle\langle\alpha\,|d\alpha=1 \tag{87}$$

We can use the completeness relation to define or change the representation of a state vector.

We can define a complex function of a real variable α, a wavefunction,

$$\psi(\alpha)=\langle\alpha|\psi\rangle \tag{88}$$

and the inner product of wavefunctions

$$\langle\psi_1|\psi_2\rangle=\int_{\alpha_{min}}^{\alpha_{max}}\psi_1^*(\alpha)\psi_2(\alpha) \tag{89}$$

Remark: The mathematical foundations of quantum mechanics are well (though slightly differently) presented in C. Cohen-Tannoudji et al., Quantum Mechanics I, Chapter II.

3 Formalism of quantum mechanics

Classically, the result of any measurement of a system of N particles can be predicted if the values of 3N coordinates and 3N momenta are known. A state of a system is known if results of all independent measurements are known.

Quantum mechanically, it is impossible to carry out simultaneous measurement of coordinate and momenta with arbitrary accuracy. A state of a quantum mechanical system is determined by the most complete measurement, i.e. simultaneous measurement of all independent physical quantities which are compatible. These quantities form the complete set of observables.

The quantities A and B are compatible if the measurement of A in no way disturbs the measurement of B. If A is compatible with B, then B is compatible with A. A and B can be measured simultaneously.

For measurements of some observables, the results form a discrete spectrum which is characteristic for a given observable of the system.

Values $\{a_1\}$, $\{a_2\}$, ... , $\{a_n\}$, ... which can be obtained for measurement of the complete set of observables $\{A\}$ are called eigenvalues of $\{A\}$.

Example: For a spinless particle the complete set of observables is given by the energy $\hat{E}$, angular momentum $\hat{l}$ and a component of angular momentum $\hat{l}_z$, $\{\hat{E}, \hat{l}, \hat{l}_z\}$. The corresponding eigenvalues form the set $\{E_j, l_j, m_j\}$.

3.1 The concept of filter

The devices defined below will allow us to present formalism of quantum theory in a unified fashion. A good example of these devices is Stern-Gerlach apparatus which is well described in C. Cohen-Tannoudji et al., Quantum Mechanics I, Chapter 4.

Separator $S_{\{A\}}$. A separator is a device such that the measurement of the complete set of observables on a system which passed through its j-th channel always gives the eigenstate $\{a_j\}$.

Recorder $R_{\{A\}}$. This devices records the channel through which the system has passed.

Measurement apparatus $M_{\{A\}}$. This apparatus consists of the separator $S_{\{A\}}$ and the recorder $R_{\{A\}}$.

Filter $F_{\sum\{a\}_j}$. The filter is a separator with shutters which close some of the channels.

3.2 Filter with ideal resolution $F_{\{a\}_j}$

A filter with ideal resolution is the filter with only one channel open.

Measurement of the complete set of observables $\{A\}$ on a system which has passed through the filter $F_{\{a\}_j}$ is the eigenvalue $\{a\}_j$. A studied system is associated with the Hilbert space $\mathcal{H}$. We assign a projector $\hat{P}_{\{a\}_j}$ to the filter $F_{\{a\}_j}$. The projector projects onto the one-dimensional subspace represented by a normalized vector $|\,\{a\}_j\rangle$:

$$\hat{P}_{\{a\}_j} = |\,\{a\}_j\rangle\langle\{a\}_j\,| \tag{90}$$

We assign a vector $|\,\{a\}_j\rangle$ to a system which has passed through the filter $F_{\{a\}_j}$. We say that a given system is in the eigenstate $\{A\}$ corresponding to the eigenvalue $\{a\}_j$, or briefly to the state $|\,\{a\}_j\rangle = |\,\{A\} = \{a\}_j\rangle$.

Eigenstates $\{A\}$ corresponding to different eigenvalues are related to different vectors and we will require these vectors to be orthogonal

$$\langle\{a\}_j|\{a\}_i\rangle = \delta_{ji} \tag{91}$$

A system prepared in a state $|\,\{a\}_i\rangle$ will pass through the filter $F_{\{a\}_j}$ iff $j = i$:

$$\hat{P}_{\{a\}_j}|\,\{a\}_i\rangle = |\,\{a\}_j\rangle\langle\{a\}_j|\{a\}_i\rangle = \delta_{ji}|\,\{a\}_j\rangle \tag{92}$$

If the system passes through the filter, the state on l.h.s. is nonzero and describes the state of the system after passage through the filter. The coefficient δ_{ji} in front of the normalized vector $|\,\{a\}_j\rangle$ on the r.h.s. is the probability that the measurement of $\{A\}$ on the state $|\,\{a\}_i\rangle$ gives the eigenvalue $\{a\}_j$.

Consider now a complete set of observables $\{B\}$ such that $\{B\} \neq \{A\}$, i.e. some observables in $\{B\}$ are incompatible with some in $\{A\}$, then for all $\{a\}_i$, the result of the measurement $\{B\}$ on the state $|\,\{a\}_i\rangle$ can not be predicted with certainty.

Now our goal will be to predict probability that a system in the state $|\,\{a\}_i\rangle$ will pass through the filter $F_{\{b\}_j}$. We first apply the relevant projector onto the initial state

$$\hat{P}_{\{b\}_j}|\,\{a\}_i\rangle = |\,\{b\}_j\rangle\langle\{b\}_j|\{a\}_i\rangle = \mathcal{A}_{\{a\}_i\to\{b\}_j}|\,\{b\}_j\rangle \tag{93}$$

Interpreting $\mathcal{A}_{\{a\}_i \to \{b\}_j} = \langle \{b\}_j | \{a\}_i \rangle$ as the desired probability (i.e. a real number) would not allow interference phenomena. These troubles disappear if we define the desired probability as

$$\mathcal{W}_{\{a\}_i \to \{b\}_j} = |\mathcal{A}_{\{a\}_i \to \{b\}_j}|^2 \tag{94}$$

The quantity $\mathcal{A}_{\{a\}_i \to \{b\}_j} = \langle \{b\}_j | \{a\}_i \rangle$ is called the probability amplitude for the transition from the state $|\,\{a\}_i\rangle$ to the state $|\,\{b\}_j\rangle$.

Important remarks.

- $\mathcal{A}_{\{a\}_i \to \{b\}_j} = \langle \{b\}_j | \{a\}_i \rangle$ implies that $\mathcal{W}_{\{a\}_i \to \{b\}_j} = \mathcal{W}_{\{b\}_j \to \{a\}_i}$, i.e. the probability to find $\{b\}_j$ when the measurement $\{B\}$ is carried out on the state $|\,\{a\}_i\rangle$ is teh same as the probability to find $\{a\}_i$ when the measurement $\{A\}$ is carried out on the state $|\,\{b\}_j\rangle$.

- The fact that some value $\{b\}_j$ will be found when measurement of $\{B\}$ is carried out is expressed as

$$\sum_j \mathcal{W}_{\{a\}_i \to \{b\}_j} = 1 \tag{95}$$

that is

$$\sum_j \langle \{a\}_i | \{b\}_j \rangle \langle \{b\}_j | \{a\}_i \rangle = 1 \tag{96}$$

and as this is valid for any ket $|\,\{a\}_i\rangle$ then

$$\sum_j |\,\{b\}_j\rangle\langle\{b\}_j\,| = 1 \tag{97}$$

This important relation is known as the completeness relation. It is essential fo mathematical structure of quantum theory and important for practical calculations. For example, it allows to write the vector $|\,\{a\}_i\rangle$ as the expansion in terms of the set $\{|\,\{b\}_j\rangle\}$

$$\begin{aligned} |\,\{a\}_i\rangle &= \sum_j |\,\{b\}_j\rangle\langle\{b\}_j|\{a\}_i\rangle = \sum_j \langle\{b\}_j|\{a\}_i\rangle |\,\{b\}_j\rangle \\ &= \sum_j \mathcal{A}_{\{a\}_i \to \{b\}_j} |\,\{b\}_j\rangle \end{aligned} \tag{98}$$

- At this point, it seems obvious to associate the probability $\mathcal{W}_{\{a\}_i \to \{b\}_j}$ with the square of the norm of the vector $\hat{P}_{\{b\}_j} |\, \{a\}_i\rangle$:

$$\mathcal{W}_{\{a\}_i \to \{b\}_j} = ||\hat{P}_{\{b\}_j} |\, \{a\}_i\rangle||^2 = \langle \{a\}_i \,|\hat{P}_{\{b\}_j} |\, \{a\}_i\rangle \tag{99}$$

  Note that here we used the idempotence of the projection operator, $\hat{P}^2 = \hat{P}$.

- Eigenstate $\{A\}$ with eigenvalue $\{a\}_i$ can be described not only by a normalized vector $|\, \{a\}_i\rangle$ but an arbitrary vector $|\, \{a\}'_i\rangle = \lambda |\, \{a\}_i\rangle$ where $\lambda \neq 0$. We then get for the probability

$$\mathcal{W}_{\{a\}_i \to \{b\}_j} = \frac{\langle \{a\}'_i \,|\hat{P}_{\{b\}_j} |\, \{a\}'_i\rangle}{\langle \{a\}'_i | \{a\}'_i\rangle} \tag{100}$$

- Vectors linearly independent on $|\, \{a\}_i\rangle$ can not be describe the eigenstate $\{A\}$ with the eigenvalue $\{a\}_i$. Let $|\, \psi\rangle \neq 0$ describes such a state, then using Eq.(100) for $\{A\} = \{B\}$, $i = j$, we get

$$\mathcal{W}_{\{a\}_i \to \{a\}_i} = \frac{|\langle \psi | \{a\}_i\rangle|^2}{\langle \psi | \psi\rangle} \leq \frac{\langle \psi | \psi\rangle \langle \{a\}_i | \{a\}_i\rangle}{\langle \psi | \psi\rangle} = 1 \tag{101}$$

  We used that $\langle \{a\}_i | \{a\}_j\rangle = \delta_{ij}$, and the Schwartz inequality $|\langle \phi | \psi\rangle| \leq ||\phi||.||\psi||$ where the equality in the last expression is valid only if $|\, \phi\rangle$ and $|\, \psi\rangle$ are linearly dependent.

  Note that when the measurement of $\{A\}$ on the system which passed through the filter $F_{\{a\}_i}$ is carried out , it always gives the eigenvalue $\{a\}_i$ with certainty: $\mathcal{W}_{\{a\}_i \to \{a\}_i} = 1$.

  In conclusion, no two linearly independent vectors in $\mathcal{H}$ can describe the same state.

3.3 Filter with finite resolution

We assign to a filter $F_{\sum\{b\}_j}$ a projector $\hat{P}_{\sum\{b\}_j}$ with the following properties

- If the system enters the filter in a state $|\, \phi\rangle$ then it will pass through with the following probability

$$\mathcal{W} = \frac{\langle \phi \,|\hat{P}_{\sum\{b\}_j} |\, \phi\rangle}{\langle \phi | \phi\rangle} \tag{102}$$

and will be in the final state

$$\hat{P}_{\sum\{b\}_j}|\,\phi\rangle \tag{103}$$

where $\hat{P}^2_{\sum\{b\}_j} = \hat{P}_{\sum\{b\}_j}$ (idempotence).

Consider first a filter with infinitely low resolution, i.e. all channels are open and it is impossible to distinguish through which the system passed through. This filter is described by an operator of identity $\hat{P}_{\sum\{b\}_j} = \sum_j |\,\{b\}_j\rangle\langle\{b\}_j\,| = \sum_j \hat{P}_{\{b\}_j}$.

- Let the initial state be $|\,\{a\}_i\rangle$, then the state after the filter is

$$|\,\psi\rangle = \hat{P}_{\sum\{b\}_j}|\,\{a\}_i\rangle \tag{104}$$

and the probability is

$$\mathcal{W}_{\{a\}_i\to\sum\{b\}_j} = \langle\{a\}_i\,|\hat{P}_{\sum\{b\}_j}|\,\{a\}_i\rangle \tag{105}$$

where

$$\mathcal{W}_{\{a\}_i\to\sum\{b\}_j} = \sum_j \mathcal{W}_{\{a\}_i\to\{b\}_j} \tag{106}$$

3.3.1 Quantum effects

Up to this point, our discussion of the formalism of quantum theory has been understandable in classical terms.Now we proceed to quantum effects and particularly the interference effect.

What is the probability that a measurement apparatus $M_{\{}C\}$ after the filter $F_{\sum\{b\}_j}$ records the value $\{c\}_k$ if the initial state was $|\,\{a\}_i\rangle$?

The state of the system after $F_{\sum\{b\}_j}$ is described by an unnormalized state $|\,\psi\rangle = \hat{P}_{\sum\{b\}_j}|\,\{a\}_i\rangle$. The probability that the result of measurement $\{C\}$ on the system in the state $|\,\psi\rangle$ will be $\{c\}_k$ is given by $||\hat{P}_{\{c\}_k}\hat{P}_{\sum\{b\}_j}|\,\{a\}_i\rangle||^2$:

$$\mathcal{W}_{\{a\}_i\to\sum\{b\}_j\to\{c\}_k} = \langle\psi\,|\hat{P}_{\{c\}_k}|\,\psi\rangle \tag{107}$$

that is

$$\begin{aligned}\mathcal{W}_{\{a\}_i\to\sum\{b\}_j\to\{c\}_k} &= |\sum_j\langle\{c\}_k|\{b\}_j\rangle\langle\{b\}_j|\{a\}_i\rangle|^2 \\ &= |\sum_j \mathcal{A}\{a\}_i\to\{b\}_j\mathcal{A}\{b\}_j\to\{c\}_k|^2 \end{aligned}\tag{108}$$

The last equation documents the origin of quantum interference effect. To provide a concrete example, we focus on the case when only two channels $\{b\}_1$ and $\{b\}_2$ are open in the filter $F_{\sum\{b\}_j}$. The probability that a measurement apparatus $M_{\{}C\}$ after the filter $F_{\{b\}_1+\{b\}_2}$ records the value $\{c\}_k$ if the initial state was $|\,\{a\}_i\rangle$ is given as

$$\begin{aligned} & \mathcal{W}_{\{a\}_i\to\{b\}_1+\{b\}_2\to\{c\}_k} = \\ = \;& |\mathcal{A}_{\{a\}_i\to\{b\}_1}\mathcal{A}_{\{b\}_1\to\{c\}_k} + \mathcal{A}_{\{a\}_i\to\{b\}_2}\mathcal{A}_{\{b\}_2\to\{c\}_k}|^2 \\ = \;& |\alpha_1\beta_1 + \alpha_2\beta_2|^2 = \\ = \;& |\alpha_1\beta_1|^2 + |\alpha_2\beta_2|^2 + 2Re(\alpha_1\beta_1\alpha_2^*\beta_2^*) \end{aligned} \tag{109}$$

where $\alpha_1 = \mathcal{A}_{\{a\}_i\to\{b\}_1}$, $\beta_1 = \mathcal{A}_{\{b\}_1\to\{c\}_k}$, $\alpha_2 = \mathcal{A}_{\{a\}_i\to\{b\}_2}$, $\beta_2 = \mathcal{A}_{\{b\}_2\to\{c\}_k}$.

If we shut of of the channels in the filter $F_{\sum\{b\}_j}$, we obtain the following probabilities

$$\mathcal{W}_{\{a\}_i\to\{b\}_1\to\{c\}_k} = |\alpha_1\beta_1|^2$$
$$\mathcal{W}_{\{a\}_i\to\{b\}_2\to\{c\}_k} = |\alpha_2\beta_2|^2$$

These terms in Eq.(109), correspond to probabilities that a classical particle will pass either through the channel $\{b\}_1$ or $\{b\}_2$. Quantum particle however passes through both channels simultaneously leading to the quantum interference effect represented by the last term in Eq(109), $2Re(\alpha_1\beta_1\alpha_2^*\beta_2^*)$. We can observe the interference effect for example in the Young double slit experiment (detailed discussion of this experiment can for example be found in Feynmann's Lectures in Physics, Vol. III, Chapter 1).

Principle of superposition and reduction of state. Let vectors $|\,\psi_1\rangle$ and $|\,\psi_2\rangle$ describe two positive states of a system, then the system can also exist in a state $|\,\psi\rangle = \alpha_1|\,\psi_1\rangle + \alpha_2|\,\psi_2\rangle$.

If we found $\{b\}_k$ by the measurement, then the system has collapsed to the state $|\,\{B\} = \{b\}_k\rangle$. This is also called reduction of a state.

3.4 Uncertainty relation

Uncertainty of a result of measuring an observable $\hat{A}$ in a given state is characterized by fluctuation $\Delta a = \sqrt{<\hat{A}^2> - <\hat{A}>^2}$, where $\Delta a = 0$ if the state is an eigenstate of $\hat{A}$.

Only compatible, i.e. commuting, observables can be measured simultaneously with arbitrary precision. Let us have two incompatible observables,

$\hat{A}$ and $\hat{B}$, with the commutation relation $[\hat{A}, \hat{B}] = i\hat{C}$. We will now derive the uncertainty relation.

We first introduce the following operators

$$\Delta\hat{A} = \hat{A} - \bar{a} \tag{110}$$
$$\Delta\hat{A} = \hat{A} - \bar{a} \tag{111}$$

where $\bar{a} = \langle\psi\,|\hat{A}|\,\psi\rangle$ and $\bar{b} = \langle\psi\,|\hat{B}|\,\psi\rangle$ and define vectors

$$|\,\phi\rangle = \Delta\hat{A}|\,\psi\rangle \tag{112}$$
$$|\,\chi\rangle = \Delta\hat{B}|\,\psi\rangle \tag{113}$$

The fluctuations of the observables $\hat{A}$ and $\hat{B}$ in the state $|\,\psi\rangle$ satisfy

$$(\Delta a)^2(\Delta b)^2 = \langle\psi\,|(\Delta\hat{A})^2|\,\psi\rangle\langle\psi\,|(\Delta\hat{B})^2|\,\psi\rangle = \|\,\phi\,\|^2\|\,\chi\,\|^2 \tag{114}$$

and according to the Schwartz inequality $\|\,\phi\,\|^2\|\,\chi\,\|^2 \geq |\langle\phi|\chi\rangle|^2$

$$\begin{aligned}\langle\phi|\chi\rangle &= \langle\psi\,|\Delta\hat{A}\Delta\hat{B}|\,\psi\rangle = \frac{1}{2}(\langle\psi\,|\{\Delta\hat{A}, \Delta\hat{B}\}|\,\psi\rangle + \langle\psi\,|[\Delta\hat{A}, \Delta\hat{B}]|\,\psi\rangle) = \\ &= \frac{1}{2}(\langle\psi\,|\{\Delta\hat{A}, \Delta\hat{B}\}|\,\psi\rangle + i\langle\psi\,|\hat{C}|\,\psi\rangle)\end{aligned} \tag{115}$$

As the operators $\hat{A}$ and $\hat{B}$ are self-adjoint operators with real eigenvalues, we can rewrite

$$|\langle\phi|\chi\rangle|^2 = \frac{1}{4}[(\langle\psi\,|\{\Delta\hat{A}, \Delta\hat{B}\}|\,\psi\rangle)^2 + (\langle\psi\,|\hat{C}|\,\psi\rangle)^2] \tag{116}$$

The inequality $\|\,\phi\,\|^2\|\,\chi\,\|^2 \geq |\langle\phi|\chi\rangle|^2$ remains satisfied if we neglect the term $\frac{1}{4}(\langle\psi\,|\{\Delta\hat{A}, \Delta\hat{B}\}|\,\psi\rangle)^2$ in the equation above. We obtain then

$$\Delta a\Delta b \geq \frac{1}{2}|\langle\psi\,|\hat{C}|\,\psi\rangle| \tag{117}$$

Example: Let $\hat{A} = \hat{X}$ and $\hat{B} = \hat{P}$, the one-dimensional coordinate and momentum operators respectively. The canonical commutation relation is $[\hat{X}, \hat{P}] = i\hbar$, so $\hat{C} = \hbar$. We define $\Delta\hat{X} = \hat{X} - x_0$ and $\Delta\hat{P} = \hat{P} - p_0$, and following the derivation above, we can easily formulate the Heisenberg uncertainty relation

$$\Delta x\Delta p \geq \frac{\hbar}{2} \tag{118}$$

In mutidimentional systems, the following holds $\Delta x_i\Delta p_j \geq \frac{\hbar}{2}\delta_{ij}$.

3.5 Energy, time and Schrödinger equation

Time evolution of quantum mechanical systems described by a state vector $|\,\psi(t)\rangle$ is governed by the Schrödinger equation

$$i\hbar\frac{d|\,\psi(t)\rangle}{dt} = \hat{H}|\,\psi(t)\rangle \tag{119}$$

where the operator $\hat{H}$ is called the Hamiltonian and represents the total energy of the system, i.e. $\hat{H} = \hat{T} + \hat{V}$ where $\hat{T}$ s the kinetic energy and $\hat{V}$ is the potential energy.

The general solution of the Schrödinger equation can be obtained by separation of variables and integration from the initial time t_0 to the final time t_f. We consider the most general case of the Hamiltonian which is explicitly time dependent, $\hat{H}(t)$,

$$\begin{aligned}
&\int_{t_0}^{t_f}\frac{d|\,\psi(t)\rangle}{|\,\psi(t)\rangle} = -\frac{i}{\hbar}\int_{t_0}^{t_f}\hat{H}(t)dt \\
&[ln(|\,\psi(t)\rangle)]_{t_0}^{t_f} = -\frac{i}{\hbar}\int_{t_0}^{t_f}\hat{H}(t)dt \\
&ln|\,\psi(t_f)\rangle - ln|\,\psi(t_0)\rangle = -\frac{i}{\hbar}\int_{t_0}^{t_f}\hat{H}(t)dt \\
&|\,\psi(t_f)\rangle = e^{-\frac{i}{\hbar}\int_{t_0}^{t_f}\hat{H}(t)dt}|\,\psi(t_0)\rangle = \hat{U}(t_0,t_f)
\end{aligned} \tag{120}$$

The operator $\hat{U}(t_0,t_f) = e^{-\frac{i}{\hbar}\int_{t_0}^{t_f}\hat{H}(t)dt}$ is the quantum evolution operator which propagates quantum mechanical system from the initial state at time t_0 to the final state at time t_f. If the Hamiltonian is not explicitely time dependent, i.e. $\hat{H} \neq \hat{H}(t)$, the expression for the evolution operator acquires a simpler form

$$\hat{U}(t_0,t_f) = e^{-\frac{i}{\hbar}\hat{H}t} \tag{121}$$

Remark: The formalism of quantum mechanics discussed in the Sec. 3 is well (though slightly differently) treated in C. Cohen-Tannoudji et al., Quantum Mechanics I, Chapter III.

4 Applications to simple quantum mechanical systems

4.1 One-particle systems

Hilbert space. Classically, to characterize a one-particle system we need three coordinates $\{x_1, x_2, x_3\}$ and three momenta $\{p_1, p_2, p_3\}$. Quantum mechanically, these are represented by self-adjoint operators $\hat{X}_j$ and $\hat{P}_j$, $j = 1, 2, 3$, such that $[\hat{X}_j, \hat{X}_k] = 0$, $[\hat{P}_j, \hat{P}_k] = 0$ and $[\hat{X}_j, \hat{P}_k] = i\hbar\delta_{jk}$. The Hilbert space will have tensor product structure $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 = h \otimes h \otimes h$ and the corresponding operators will become

$$\begin{aligned} \hat{X}_1 &= \hat{X} \otimes \hat{1} \otimes \hat{1}, \hat{P}_1 = \hat{P} \otimes \hat{1} \otimes \hat{1}, \\ \hat{X}_2 &= \hat{1} \otimes \hat{X} \otimes \hat{1}, \hat{P}_1 = \hat{1} \otimes \hat{P} \otimes \hat{1}, \\ \hat{X}_3 &= \hat{1} \otimes \hat{1} \otimes \hat{X}, \hat{P}_1 = \hat{1} \otimes \hat{1} \otimes \hat{P} \end{aligned}$$

where $\hat{1}$ is an identity operator and the self-adjoint operators $\hat{X}$ and $\hat{P}$ are defined so that they satisfy the canonical commutation relation $[\hat{X}, \hat{P}] = i\hbar$. The values of $\hat{X}$ are continuous and from $(-\infty, \infty)$.

The most suitable Hilbert space on which these conditions for $\hat{X}$ are satisfied is the one on which the operator $\hat{X}$ forms a complete set of commuting operators $h = L^2(\mathbb{R})$. This Hilbert space is formed by all complex functions $A(\xi)$ of a real variable ξ for which there exists a (Lebesgue) integral $\int_{-\infty}^{\infty} |A(\xi)|^2 d\xi < \infty$.

Let us have the vectors $|\, A\rangle, |\, B\rangle \in L^2(\mathbb{R})$, where $|\, A\rangle = A(\xi)$ and $|\, B\rangle = B(\xi)$ are square integrable functions $\int_{-\infty}^{\infty} |A(\xi)|^2 d\xi < \infty$ and $\int_{-\infty}^{\infty} |B(\xi)|^2 d\xi < \infty$ (meaning their norm is finite). The linear combination of these vectors is defined as $\alpha|\, A\rangle + \beta|\, B\rangle = \alpha A(\xi) + \beta B(\xi)$, and the inner product is defined as

$$\langle A|B\rangle = \int_{-\infty}^{\infty} A^*(\xi) B(\xi) d\xi \tag{122}$$

Coordinate and momentum representations. The spectral representation of $\hat{X}$ is given as

$$\hat{X} = \int_{-\infty}^{\infty} x|\, x\rangle\langle x\, | dx \tag{123}$$

and the completeness relation is

$$\hat{X} = \int_{-\infty}^{\infty} |\, x\rangle\langle x\, | dx = 1 \tag{124}$$

Every vector $|\,\phi\rangle \in h$ is in the coordinate representation (or X-representation) described by a wavefunction

$$\phi(x) = \langle x|\phi\rangle \tag{125}$$

which are coefficients in the expansion of the vector $|\,\phi\rangle$ in terms of the eigenstates of the operator $\hat{X}$: $|\,\phi\rangle = \int_{-\infty}^{\infty} |\,x\rangle\langle x|\phi\rangle dx = \int_{-\infty}^{\infty} \phi(x)|\,x\rangle dx$.

For $|\,\phi\rangle_1, |\,\phi\rangle_2 \in h$, the inner product is defined as

$$\langle\phi_1|\phi_2\rangle = \int_{-\infty}^{\infty} \phi_1^*(x)\phi_2(x)dx \tag{126}$$

The operator $\hat{P}$ has to satisfy the canonical commutation relation $[\hat{X}, \hat{P}] = i\hbar$, i.e. $\hat{X}\hat{P}|\,\phi\rangle - \hat{P}\hat{X}|\,\phi\rangle = i\hbar|\,\phi\rangle$. In the coordinate representation, this is

$$x\hat{P}^{(X)}\phi(x) - \hat{P}^{(X)}x\phi(x) = i\hbar\phi(x) \tag{127}$$

which is satisfied by

$$\hat{P}^{(X)} = -i\hbar\frac{d}{dx} \tag{128}$$

This operator is self-adjoint.

For $\forall p \in \mathbb{R}$, there is a solution of the equation

$$-i\hbar\frac{d}{dx}\psi_p(x) = p\psi_p(x) \tag{129}$$

and every solution linearly depends on function

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}px} \tag{130}$$

which satisfies the normalization condition

$$\int_{-\infty}^{\infty} \psi_{p'}^*(x)\psi_p(x)dx = \delta(p - p') \tag{131}$$

Similarly

$$\int_{-\infty}^{\infty} \psi_p^*(x')\psi_p(x)dx = \delta(x - x') \tag{132}$$

$\psi_p(x)$ is an eigenfunction of $\hat{P}$ in the coordinate representation corresponding to the eigenvalue p. The completeness relation is

$$\int_{-\infty}^{\infty} |\,p\rangle\langle p\,|dp = 1 \tag{133}$$

and the spectral representation of $\hat{P}$ is

$$\hat{P} = \int_{-\infty}^{\infty} p|\, p\rangle\langle p\,|dp \tag{134}$$

Every vector $|\,\phi\rangle \in h$ in the momentum representation (or P-representation) corresponds to the wavefunction

$$\phi^{(P)}(p) = \langle p|\phi\rangle \tag{135}$$

where

$$\phi^{(P)}(p) = \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|\phi\rangle dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}px}\phi(x)dx \tag{136}$$

This relation shows that the wavefunction $\phi^{(P)}(p)$ which describes the vector $|\,\phi\rangle$ in the momentum representation is related to $\phi(x)$ which describes the same vector in the coordinate representation by the Fourier transform.

Let us have specially $|\,\phi\rangle = \hat{X}|\,\psi\rangle$,

$$\begin{aligned} \hat{X}^{(P)}\psi^P(x) &= \langle p\,|\hat{X}|\,x\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}px}\langle x\,|\hat{X}|\,\psi\rangle dx = \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}px} x\psi(x)dx \\ &= \frac{i\hbar}{\sqrt{2\pi\hbar}} \frac{d}{dp} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}px}\psi(x)dx \end{aligned} \tag{137}$$

that is

$$\hat{X}^{(P)}\psi^P(x) = i\hbar\frac{d}{dp}\psi^P(x) \tag{138}$$

In the momentum representation, the operator $\hat{X}$ is therefore defined as $\hat{X}^{(P)} = i\hbar\frac{d}{dp}$.

Schrödinger equation in coordinate representation. So far we have dealt with the Hamiltonian (in the context of time evolution) on an abstract operator level (end of the Sect. 3). Now we would like to arrive to a concrete form and representation of the Hamiltonian. We start from a classical Hamiltonian, which we will quantize by using the correspondence principle, i.e. we assign relevant quantum operators to classical variables. The classical Hamiltonian has the following form

$$H(\vec{x},\vec{p}) = \frac{\vec{p}^2}{2m} + V(\vec{x}) \tag{139}$$

where the first term represents the kinetic energy and the second term is the potential energy. By assigning the operator $\hat{\vec{X}}$ to the classical coordinate $\vec{x}$ and the operator $\hat{\vec{P}}$ to the classical momentum $\vec{p}$, we obtain (note that we deal in general with three-dimensional case)

$$\hat{H} = \frac{\hat{\vec{P}}}{2m} + V(\hat{\vec{X}}) \tag{140}$$

In order to proceed to the coordinate representation, we apply the canonical quantization, that is, we perform the following substitutions

$$\hat{\vec{X}} \to \vec{x} \tag{141}$$

$$\hat{\vec{P}} \to -i\hbar \sum_{j=1}^{3} \frac{\partial^2}{\partial x_j^2} = -i\hbar\Delta \tag{142}$$

The quantum Hamiltonian in the coordinate representation then becomes

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(\hat{\vec{X}}) \tag{143}$$

In the special case that the potential energy $V(\hat{\vec{X}}) = 0$, we say that the Hamiltonian describes a free particle.

4.2 Fourier transform

Our presentation of the Fourier transform followed C. Cohen-Tannoudji et al., Quantum Mechanics II, Appendix I.

4.3 δ function

C. Cohen-Tannoudji et al., Quantum Mechanics II, Appendix II.

4.4 Free particle

C. Cohen-Tannoudji et al., Quantum Mechanics I, Chapter I, Sections B and C.

4.5 Particle in time-independent scalar potential

C. Cohen-Tannoudji et al., Quantum Mechanics I, Chapter I, Section D and Appendix H_I.

4.6 One-dimensional harmonic oscillator

C. Cohen-Tannoudji et al., Quantum Mechanics I, Chapter V.

Remark: Please note the the lecture notes may contain typos. It would be appreciated if you let me know in the case you find any. Also, if there is anything you consider unclear or incomplete, or if you have any questions regarding the notes please do not hesitate to contact me.