Chapter 1: Fundamental concepts

In this chapter we summarize the most important definitions and concepts that are relevant to quantum mechanics. Much of the material that follows is quite elementary and is probably well known to graduate students. We discuss it mainly to establish a common language and notation.

1-1- The Hilbert space, Dirac notation and Wavefunction

In quantum mechanics the physical state of a system is represented by elements (vectors), these elements are called state vectors. State vectors are part of linear vector space that we call a **Hilbert space** $\mathcal{H}$. Dirac introduced a powerful formalism referred to as Dirac notation or bra-ket notation, in which the state vector ϕ is denoted by the symbol $|\phi\rangle$, which he called a ket vector, or simply a ket. Kets belong to the Hilbert space $\mathcal{H}$, or, in short, to the ket space. Dirac denoted the elements ϕ^* of the Hilbert space $\mathcal{H}$ by the symbol $\langle\phi|$, which he called a bra vector, or simply a bra. Bra vectors are elements of a vector space, called dual space $\mathcal{H}^*$ of the original Hilbert space $\mathcal{H}$. Thus:

- The scalar product of the vectors ϕ_1 and ϕ_2 is:

$$(\phi_1,\phi_2)=\langle\phi_1|\phi_2\rangle \qquad \text{......(1-1-1)}$$

Where, we have to note that eq. (1-1-1) satisfy:

$$\langle\phi_1|\phi_2\rangle^*=\langle\phi_2|\phi_1\rangle \qquad \text{......(1-1-2)}$$

The scalar product in quantum mechanics is generally referred to as an **inner product** or a **projection**.

- Two ket states ϕ_1 and ϕ_2, are said to be orthonormal if they are orthogonal and if each one of them has a unit norm:

$$\langle\phi_1|\phi_2\rangle=0 \quad , \quad \langle\phi_1|\phi_1\rangle=1 \quad , \quad \langle\phi_2|\phi_2\rangle=1 \qquad \text{......(1-1-3)}$$

- Any linear combination of a set of vectors ($|\phi_1\rangle$, $|\phi_2\rangle$, …, $|\phi_N\rangle$), is also a vector of the same space, i.e. $a|\phi_1\rangle+b|\phi_2\rangle+\cdots+q|\phi_N\rangle$.

- The set of vectors, ($|\phi_1\rangle$, $|\phi_2\rangle$, …, $|\phi_N\rangle$), to be denoted in short by $\{|\phi_i\rangle\}$, are called the basis of the vector space, and the basis set satisfies the orthonormality condition:

$$\langle \phi_i | \phi_j \rangle = \delta_{ij} \qquad \text{......(1-1-4)}$$

- The dimension of a vector space is given by the maximum number of linearly independent vectors the space can have. For instance, if the maximum number of linearly independent vectors a space has is N (i.e., $|\phi_1\rangle$, $|\phi_2\rangle$, …, $|\phi_N\rangle$), such space is said to be of N-dimensional.

- The basis set is said to be complete if it spans the entire Hilbert space of the system under consideration. This means that any state vector $|\Psi\rangle$ (or wavefunction) in the Hilbert space can be expressed as a linear superposition of the basis vectors,

$$|\Psi\rangle = \sum_{i=1}^{N} c_i |\phi_i\rangle \qquad \text{......(1-1-5)}$$

Where, the expansion coefficients c_i in (1-1-5) are called the components of the vector $|\Psi\rangle$ in the basis. Each component is given by the scalar product of $|\Psi\rangle$ with the corresponding base vector,

$$c_i = \langle \phi_i | \Psi \rangle \qquad \text{......(1-1-6)}$$

- In wave mechanics we deal with wave functions $\Psi(\vec{r},t)$, but in the more general formalism of quantum mechanics we deal with abstract kets $|\Psi\rangle$. Although, wave functions, like kets, are elements of a Hilbert space but kets do not have any spatial dependence as wave functions do. Of course, if we want to know the probability of finding the particle at some position in space, we need to work out the formalism within the coordinate representation. In the coordinate representation, the scalar product $\langle \Psi | \Phi \rangle$ is given by

$$\langle \Psi | \Phi \rangle = \int \Psi^*(\vec{r},t)\Phi(\vec{r},t)d\tau \qquad \text{......(1-1-7)}$$

A function $\Psi(\vec{r})$ is said to be square integrable if the scalar product of $\Psi(\vec{r},t)$ with itself

$$\langle \Psi | \Psi \rangle = \int |\Psi^*(\vec{r},t)|^2 d\tau \qquad \text{......(1-1-8)}$$

is finite. In 1927 Born interpreted $|\Psi(\vec{r},t)|^2 = \rho(\vec{r},t)$ as the probability density and $|\Psi(\vec{r},t)|^2 d\tau$ as the probability of finding a particle at time t in the volume element $d\tau$ located between $\vec{r}$ and $\vec{r}+d\vec{r}$. Thus, the total probability of finding the particle somewhere in space must be equal to one: i.e.

$$\langle \Psi | \Psi \rangle = \int |\Psi^*(\vec{r},t)|^2 d\tau = 1 \qquad \text{(Normalization condition)} \qquad \text{......(1-1-9)}$$

Ex. Consider two states $|\psi_1\rangle = 2i|\phi_1\rangle + |\phi_2\rangle - a|\phi_3\rangle + 4|\phi_4\rangle$ and $|\psi_2\rangle = 3|\phi_1\rangle - i|\phi_2\rangle + 5|\phi_3\rangle - |\phi_4\rangle$ where $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$, and $|\phi_4\rangle$ are orthonormal kets and where "a" is constant. Find the value of "a" so that $|\psi_1\rangle$ and $|\psi_2\rangle$ are orthogonal.

Soln.

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

$$\left(3\langle\phi_1| + i\langle\phi_2| + 5\langle\phi_3| - \langle\phi_4|\right)\ \left(2i|\phi_1\rangle + |\phi_2\rangle - a|\phi_3\rangle + 4|\phi_4\rangle\right) = 6i + i - 5a - 4 = 0 \quad \rightarrow \quad a = (7i - 4)/5$$

1-2- Hermitian operators

An operator $\hat{Q}$ is a mathematical rule that when applied to a ket $|\psi\rangle$ transforms it into another ket $|\psi'\rangle$ of the same space and when it acts on a bra $\langle\Phi|$ transforms it into another bra $\langle\Phi'|$

$$\hat{Q}|\psi\rangle = |\psi'\rangle, \qquad \langle\Phi|\hat{Q} = \langle\Phi'| \qquad \text{……(1-2-1)}$$

When an operator $\hat{Q}$ is sandwiched between a bra $\langle\Phi|$ and a ket $|\psi\rangle$, it yields in general a complex number, i.e. $\langle\Phi|\hat{Q}|\psi\rangle$= complex number. The quantity $\langle\Phi|\hat{Q}|\psi\rangle$ can also be a purely real or a purely imaginary number. It does not matter if one first applies $\hat{Q}$ to the ket and then takes the bra-ket or one first applies $\hat{Q}$ to the bra and then takes the bra-ket; that is

$$\left(\langle\Phi|\hat{Q}\right)|\psi\rangle = \langle\Phi|\left(\hat{Q}|\psi\rangle\right) \qquad \text{……(1-2-2)}$$

- The Hermitian adjoint or simply the adjoint, $\alpha^\dagger$ of a complex number α is the complex conjugate of this number: $\alpha^\dagger = \alpha^*$.
- The Hermitian adjoint, $\hat{Q}^\dagger$, of an operator $\hat{Q}$ is defined by this relation:

$$\langle\psi|\hat{Q}^\dagger|\Phi\rangle = \langle\Phi|\hat{Q}|\psi\rangle^* \qquad \text{……(1-2-3)}$$

- An operator $\hat{Q}$ is said to be Hermitian, if it is equal to its adjoint $\hat{Q}^\dagger$:

$$\hat{Q} = \hat{Q}^\dagger \quad \text{or} \quad \langle\psi|\hat{Q}|\Phi\rangle = \langle\Phi|\hat{Q}|\psi\rangle^* \qquad \text{……(1-2-4)}$$

- If an operator is Hermitian, then an operator can act to the right on a ket or to the left on a bra with the same result, i.e.,

$$\hat{Q}|\psi\rangle = |\psi'\rangle \quad \text{and} \quad \langle\psi|\hat{Q} = \langle\psi'| \qquad \text{......(1-2-5)}$$

- An operator $\hat{Q}$ is said to be skew-Hermitian or anti-Hermitian if,

$$\hat{Q}^{\dagger} = -\hat{Q} \quad \text{or} \quad \langle\psi|\hat{Q}|\Phi\rangle = -\langle\Phi|\hat{Q}|\psi\rangle^{*} \qquad \text{......(1-2-6)}$$

- In quantum mechanics, all operators that correspond to physical observables are Hermitian. Hermitian operator has the following properties:

1- The eigenvalues of Hermitian operator are all real and the eigenvectors corresponding to different eigenvalues are orthogonal. **(prove)**.

2- Hermitian operator in an N-dimensional Hilbert space has N distinct eigenvalues (i.e. no degeneracy), then its eigenvectors $|\phi_n\rangle$ form complete set of vectors (i.e. a complete basis set). Any admissible state vector $|\psi\rangle$ can be expanded in terms of eigenvectors of such Hermitian operator, i.e.,

$$|\psi\rangle = \sum_{n=1}^{N} c_n |\phi_n\rangle \qquad \text{......(1-2-7)}$$

H.W. Check whether the following operators are Hermitian or not: the linear momentum operator $\hat{p}_x$, position operator $\hat{x}$, $\frac{d}{dx}$ and $i\frac{d}{dx}$.

1-3- Eigenvalue problem and Expectation values

A state vector $|\phi\rangle$ is said to be an eigenvector (also called an eigenket) of an operator $\hat{A}$ if the application of $\hat{A}$ on $|\phi\rangle$ gives:

$$\hat{A}|\phi\rangle = a|\phi\rangle \qquad \text{......(1-3-1)}$$

where "a" is a complex number, called an eigenvalue of $\hat{A}$. Equation (1-3-1) is known as the eigenvalue equation, or eigenvalue problem, of the operator $\hat{A}$. The only possible result of a measurement is one of the eigenvalues associated with the corresponding eigenstates of an observable.

- If the system is in any other state, say $|\psi\rangle$ which is not an eigenstate of the considered operator, then the possible outcomes of the measurement cannot be predicted precisely, therefore to determine the observable associated with $\hat{A}$, one has to use the expectation value (average value) defined as:

$$\langle\hat{A}\rangle = \frac{\langle\psi|\hat{A}|\psi\rangle}{\langle\psi|\psi\rangle} \qquad \text{……(1-3-2)}$$

- If the system is in a superposition of eigenstates, e.g., $|\psi\rangle = \sum_n c_n |\phi_n\rangle$, the expectation value is a weighted average of the eigenvalues:

$$\langle\hat{A}\rangle = \sum_n |c_n|^2 a_n = \sum_n a_n P_n \qquad \text{……(1-3-3)}$$

Where we have used $\langle\phi_m|\hat{A}|\phi_n\rangle = a_n\delta_{nm}$

The quantity $P_n = |c_n|^2$ represents the probability of finding the value “a_n“ after measuring the observable A.

Ex. Imagine a quantum system with an observable A that has three possible measurement results: a_1, a_2, and a_3. The three kets $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$ corresponding to these possible results form a complete orthonormal basis. The system is prepared in the state $|\psi\rangle = 2|\phi_1\rangle - 3|\phi_2\rangle + 4i|\phi_3\rangle$. Calculate the probabilities of all possible measurement results of the observable A.

Soln.

$$\langle\psi|\psi\rangle = C^*\left(2\langle\phi_1| - 3\langle\phi_2| - 4i\langle\phi_3|\right)C\left(2|\phi_1\rangle - 3|\phi_2\rangle + 4i|\phi_3\rangle\right) = 1$$

$$1 = |C|^2\, 29 \;\rightarrow\; C = \frac{1}{\sqrt{29}}$$

The normalized state is: $|\psi\rangle = \frac{1}{\sqrt{29}}\left(2|\phi_1\rangle - 3|\phi_2\rangle + 4i|\phi_3\rangle\right)$

The probabilities of measuring the results a_1, a_2, and a_3 are

$P(a_1) = |\langle\phi_1|\psi\rangle|^2 = \frac{4}{29}$, $P(a_2) = |\langle\phi_2|\psi\rangle|^2 = \frac{9}{29}$ and $P(a_3) = |\langle\phi_3|\psi\rangle|^2 = \frac{16}{29}$, respectively.

1-4- Commuting operators

The commutator of two operators $\hat{A}$ and $\hat{B}$, denoted by $[\hat{A},\hat{B}]$, is defined by:

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \qquad \text{……(1-4-1)}$$

and the anti-commutator $\{\hat{A},\hat{B}\}$ is defined by

$$\{\hat{A},\hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A} \qquad \text{……(1-4-2)}$$

Two operators are said to commute if their commutator is equal to zero and hence

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0 \quad \rightarrow \quad \hat{A}\hat{B} = \hat{B}\hat{A} \qquad \text{……(1-4-3)}$$

Thus, for commuting operators the order of operation does not matter, whereas it does for non-commuting. Two observables A and B are said to be compatible when their corresponding operators commute, $[\hat{A},\hat{B}] = 0$; observables corresponding to non-commuting operators are said to be non-compatible

If two observables are compatible, their corresponding operators possess a set of common (or simultaneous) eigenstates (this holds for both degenerate and nondegenerate eigenstates). So compatible observables can be measured simultaneously with arbitrary accuracy; non-compatible observables cannot.

H.W. Show that the operators $\hat{x}$ and $\hat{p}_x$ don't commute.

H.W. Prove, **i**f there exists a common (simultaneous) complete set of eigenfunctions for two linear operators, then the operators commute.

H.W. Consider the states $|\psi\rangle = 3i|\chi_1\rangle - 7i|\chi_2\rangle$ and $|\Phi\rangle = -|\chi_1\rangle + 2i|\chi_2\rangle$, where $|\chi_1\rangle$ and $|\chi_2\rangle$ are orthonormal.

(a) Calculate $|\psi + \Phi\rangle$ and $\langle\psi + \Phi|$.

(b) Calculate the scalar products $\langle\psi|\Phi\rangle$ and $\langle\Phi|\psi\rangle$. Are they equal?

1-5- Uncertainty principle

The spread of the measured result from the average is known as the deviation. The uncertainty (variance) is defined as the root-mean-square of the deviation. The uncertainty of an observable "A"

$$\Delta A = \sqrt{\left\langle \left(A - \langle A \rangle\right)^2 \right\rangle} = \sqrt{\left\langle A^2 \right\rangle - \langle A \rangle^2} \qquad \text{……(1-5-1)}$$

The connection between the commutator of two operators $\hat{A}$ and $\hat{B}$, and the possible uncertainty of measurements of the two corresponding observables can be deduced from the quantum mechanical generalized uncertainty relation:

$$\Delta A \Delta B \geq \frac{1}{2}\left|\left\langle \left[\hat{A}, \hat{B}\right] \right\rangle\right| \qquad \text{……(1-5-2)}$$

Its application to position “x” and momentum “p_x” observables leads to $\Delta x \Delta p_x \geq \frac{\hbar}{2}$, which indicates, that if the x-component of the momentum of a particle is measured with an uncertainty Δp_x , then the uncertainty Δx associated with its position “x” measurement cannot be smaller than $\hbar / 2\Delta p_x$. The three-dimensional form of the uncertainty relations for position and momentum can be written as follows:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}\ , \qquad \Delta y \Delta p_y \geq \frac{\hbar}{2}\ , \qquad \Delta z \Delta p_z \geq \frac{\hbar}{2} \qquad \text{……(1-5-3)}$$

Uncertainty is inherent and fundamental, meaning that one cannot design the experiment any better to improve the result, and indicates that, although it is possible to measure the momentum or position of a particle accurately, it is not possible to measure these two observables simultaneously to an arbitrary accuracy.
Heisenberg’s uncertainty principle can be generalized to any pair of complementary, or canonically conjugate, dynamical variables: *it is impossible to devise an experiment that can measure simultaneously two complementary variables to arbitrary accuracy (if this were ever achieved, the theory of quantum mechanics would collapse).*
Energy and time, for instance, form a pair of complementary variables. Their simultaneous measurement must obey the time–energy uncertainty relation:

$$\Delta E \Delta t \geq \frac{\hbar}{2} \qquad \text{……(1-5-4)}$$

This relation states that if we make two measurements of the energy of a system and if these measurements are separated by a time interval Δt, the measured energies will differ by an amount ΔE which can in no way be smaller than $\hbar / 2\Delta t$.