PHYS-453

2-BASIC MATHEMATICAL CONCEPTS

…and their role in QM

Average value-a

Consider a statistical quantity A for which all the possible values make up a discrete sequence a_1, a_2, …a_n,… and in a set of N measurements they turn up N_1, N_2, …N_n,…times. Then, the average value is given by

$$\langle A \rangle = \frac{N_1 a_1 + N_2 a_2 + \ldots N_n a_n + \ldots}{N} = \sum_n a_n f_n \qquad (2.1)$$

Average value-b

In the limit where $N \rightarrow \infty$ the frequencies f_n tend to the probabilities of P_n appearance of the values a_n, thus

$$\langle A \rangle = \sum_n a_n P_n \qquad (2.2)$$

Thus the average value of a statistical quantity is the sum of its possible values multiplied by the corresponding probability

Average value-c

For a generic function *G(A)* of the statistical quantity *A* the average value is given by

$$\left\langle G(A) \right\rangle = \sum_n G\left(a_n\right)P_n \qquad (2.3)$$

All the previous discussion is valid when the "spectrum" of the possible values is discrete. What is going on when is is continuous? That is, when the quantity *A* can get all possible values within a range?

Average value-d

In this case we introduce the density probability *P(a)*. The product *P(a)da* gives the probability of finding the values of quantity *A* in the range between *a* and *a* +*da*. The average value of *A* is given by

$$\langle A \rangle = \sum_a aP(a) \equiv \int_{-\infty}^{+\infty} aP(a)\, da \qquad (2.4)$$

Similarly for a function *G(A)* of *A*

$$\langle G(A) \rangle = \int_{-\infty}^{+\infty} G(a)P(a)\, da \qquad (2.5)$$

Standard Deviation or Uncertainty

- The standard deviation or uncertainty of a statistical quantity *A* is given by

$$(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 \qquad (2.6)$$

where we have the following

$$\langle A^2 \rangle = \sum_n a_n^2 P_n \qquad (2.7)$$

Discrete distribution

$$\langle A^2 \rangle = \int a^2 P(a) da \qquad (2.8)$$

Continuous distribution

The Linear Operators-a

- With the term *operator*, we actually mean the mapping of a set of mathematical objects on another set (which is normally the original one). For example when we differentiate a function we map it on another function (the derivative). In this case we talk about an operator *D* for which,

$$\hat{D} = \frac{d}{dx} : \quad \rightarrow \quad \hat{D} f(x) = \frac{d}{dx} f(x)$$

The Linear Operators-b

- The operators which we use in quantum mechanics are *linear*.

$$\hat{A}\left(c_1\psi_1 + c_2\psi_2\right) = c_1\left(\hat{A}\psi_1\right) + c_2\left(\hat{A}\psi_2\right) \quad (2.9)$$

- The operator algebra has the following properties:

$$\left(\hat{A} + \hat{B}\right)\psi = \hat{A}\psi + \hat{B}\psi, \qquad \left(\hat{A}\cdot\hat{B}\right)\psi = \hat{A}\left(\hat{B}\psi\right)$$

$$\hat{A}\cdot\hat{B} \neq \hat{B}\cdot\hat{A} \quad (2.10)$$

The Linear Operators-c

- In the case where $\hat{A} \cdot \hat{B} = \hat{B} \cdot \hat{A}$ we say that the two operators **commute**.
- The quantity $\left[\hat{A}, \hat{B}\right] = \hat{A} \cdot \hat{B} - \hat{B} \cdot \hat{A}$ is called the **commutator**.
- Two operators are said to be equal when their action on a generic function gives the same result:

$$\hat{A} = \hat{B} \Leftrightarrow \hat{A}\psi = \hat{B}\psi \qquad (2.11)$$

Properties of commutators

$$\left[\hat{A},\ \hat{B}\right] = -\left[\hat{B},\ \hat{A}\right]$$

$$\left[\hat{A},\ \hat{B}+\hat{C}\right] = \left[\hat{A},\ \hat{B}\right]+\left[\hat{A},\ \hat{C}\right]$$

$$\left[\hat{A}\cdot\hat{B},\ \hat{C}\right] = \hat{A}\cdot\left[\hat{B},\ \hat{C}\right]+\left[\hat{A},\ \hat{C}\right]\cdot\hat{B}$$

$$\left[\hat{A},\ \hat{B}\cdot\hat{C}\right] = \hat{B}\cdot\left[\hat{A},\ \hat{C}\right]+\left[\hat{A},\ \hat{B}\right]\cdot\hat{C}$$

$$\left[\hat{A},\ \mathrm{c}\hat{B}\right] = c\left[\hat{A},\ \hat{B}\right] = \left[c\hat{A},\ \hat{B}\right]$$

$$\left[\hat{A},\ \hat{A}\right] = \left[\hat{A},\ \hat{A}^{n}\right] = \left[\hat{A},\ f(\hat{A})\right] = \left[\hat{A},\ c\right] = 0 \quad (2.12)$$

Eigenvalues and Eigenfunctions of Operators -a

- For the operators used in quantum mechanics there are functions such that when the operator is applied on them it simply multiplies them with a real number *a*.

$$\hat{A}\psi = a\psi$$

- The functions ψ are called **eigenfunctions** of the operator and the real numbers *a* are called **eigenvalues** of the operator.

Eigenvalues and Eigenfunctions of Operators –b

- If the eigenvalues can take any real value we say that the operator's spectrum is **continuous**. On the contrary if they take only certain real values then the operator's spectrum is **discrete**.
- If for a given eigenvalue we have more than one eigenfunction then the spectrum is called **degenerate**.

Dirac formalism: a new way for representing wave functions-a

- According to Dirac, any quantum state ψ is represented by two vectors: The first is a column vector, is denoted as $|\psi\rangle$, and is called ***ket vector***. The second is a row vector and is denoted by $\langle\psi|$ and is called ***bra vector***. These names come from the English word bracket because in this formalism the dot product of two states ψ and ϕ is given by

$$\int_{-\infty}^{+\infty} \psi^*(x)\phi(x)\,dx = (\psi,\phi) = \langle\psi|\phi\rangle \qquad (2.13)$$

Dirac formalism: a new way for representing wave functions-b

- With this formalism the average value of a physical quantity on a state ψ is denoted by:

$$\left\langle A \right\rangle = \int_{-\infty}^{\infty} \psi^*\left(x\right)\left(A\psi\left(x\right)\right)dx = \left\langle \psi \middle| A \middle| \psi \right\rangle \qquad (2.14)$$

- The two vectors are related by the following relations

$$\left(\left|\psi\right\rangle\right)^{\dagger} = \left\langle\psi\right|, \quad \left(\left\langle\psi\right|\right)^{\dagger} = \left|\psi\right\rangle \qquad (2.15)$$

$$\left(c_1\left|\psi_1\right\rangle + c_2\left|\psi_2\right\rangle\right)^{\dagger} = c_1^*\left\langle\psi_1\right| + c_2^*\left\langle\psi_2\right| \quad (2.16)$$

The dot product

- The dot product of two square integrable functions ψ and ϕ is denoted and defined by:

$$\langle\psi|\phi\rangle = \int_{-\infty}^{+\infty} \psi^*(x)\phi(x)dx \qquad (2.17)$$

- The dot product has the following properties:

$$\langle\psi|\psi\rangle \geq 0, \qquad \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$$
$$\langle\psi|c|\phi\rangle = \langle\psi|c\phi\rangle = c\langle\psi|\phi\rangle, \quad c \in \mathrm{C} \qquad (2.17)$$
$$\langle\psi|\phi_1 + \phi_2\rangle = \langle\psi|\phi_1\rangle + \langle\psi|\phi_2\rangle$$

Conjugate states in Dirac formalism

- In Dirac formalism when we have to consider conjugate states we must take into account the following:

$$\left|\phi\right\rangle = c\left|\psi\right\rangle \Leftrightarrow \left\langle\phi\right| = c^{*}\left\langle\psi\right|$$
$$\left|\phi\right\rangle = \hat{A}\left|\psi\right\rangle \Leftrightarrow \left\langle\phi\right| = \left\langle\psi\right|\hat{A}^{\dagger} \quad (2.18)$$

- Where $\hat{A}^{\dagger}$ is the conjugate operator of $\hat{A}$

Self-adjoint or Hermitian Operator

- When $\hat{A}^\dagger = \hat{A}$ the operator is called **self-adjoint** or **Hermitian**. For such an operator we have:

$$\left|\phi\right\rangle = \hat{A}\left|\psi\right\rangle \Leftrightarrow \left\langle\phi\right| = \left\langle\psi\right|\hat{A}^\dagger = \left\langle\phi\right| = \left\langle\psi\right|\hat{A} \quad (2.19)$$

- A Hermitian operator has: a) real eigenvalues b) real average value c) orthogonal eigenstates d) for all the previous it is proper for representing physical quantities.

Hermitian Operator a Definition

- We say that a linear operator $\hat{A}$, which acts on a functional space, is hermitian if for any couple of functions $\psi(x)$, $\phi(x)$ the following relation holds:

$$\int \psi^* \left(A\phi\right) dx = \int \left(A\psi\right)^* \phi dx \qquad (2.20)$$

- In other words the action can be transferred – without change of the result between the functions of the integral.

Properties of Hermitian Operators

- If $\hat{A}, \hat{B}$ are Hermitian operators then the following operators are Hermitian as well:

$$\hat{A}+\hat{B}, \quad \hat{A}^n, \quad \lambda\hat{A}$$

- The operator $\hat{A}\cdot\hat{B}$ is Hermitian only if the two operators commute, i.e. $\hat{A}\cdot\hat{B}=\hat{B}\cdot\hat{A}$.
- The eigenfunctions of a Hermitian operator form a **complete orthonormal basis** in the space of the physical states. This means that any wave function can be expressed as a linear combination of the operator's eigenfunctions.

Projection and Parity Operators

- An operator $\hat{P}$ is called a **projection operator** when it is Hermitian and is equal to its square:

$$\hat{P}^2 = \hat{P} \qquad (2.21)$$

- The **parity** operator reflects the position vector **r** in the expression of a function:

$$\hat{P}\psi(\mathbf{r}) = \psi(-\mathbf{r}) \qquad (2.22)$$