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Revisiting Expectation Values in Quantum Mechanics

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Abstract - Quantum mechanics is a relatively new branch of physics as compared to the other branches. Many of its concepts are a bit confusing, which is quite obvious, because it completely destroys the classical intuitions of physicists as well as students. But some of its concepts have a classical mechanical analogy and one such concept is the concept of expectation value of observables or operators in quantum mechanics. In a way it is related to the concept of centre of mass in classical mechanics. So, in this paper, first, a review of this concept and its correspondence with centre of mass and later the reason behind the naming of this concept is discussed in brief.

Keywords - Expectation value, Weighted average, Centre of mass

I. INTRODUCTION

In quantum mechanics to every physically measurable quantity, called as *"Observable"* or dynamical variable, there corresponds an *"Operator"*. Examples of such observable are position, momentum & energy, etc. The measurement of an observable in a quantum mechanical system is mathematically represented by the action of its corresponding operator on a wave function, which represents the state of that quantum mechanical system. The measurement of an observable involves a large number of observations with the same wave function since quantum mechanical systems are probabilistic in nature and one observation is not enough to find out the true value of the observable accurately. If we want to measure an observable A, then the outcomes of different observations will be, in general, different, i.e., a_1, a_2, a_3 and so on. A special type of average of all such values of A is known as the **Expectation value** of the operator $\hat{A}$, associated with observable A and it's expressed as [1]

$$\langle \hat{A} \rangle = \frac{\iiint \Psi^* \hat{A}\ \Psi\ d^3r}{\iiint \Psi\ \Psi^*\ d^3r} \tag{1}$$

Where,
$\langle \hat{A} \rangle$ = Expectation value of operator $\hat{A}$,
Ψ = wave function representing the state of the system,
Ψ^* = complex conjugate of that wave function,
d^3r = volume element in 3D.
Now let's understand the meaning of this equation and that special type of average as mentioned above.

II. AVERAGE VS. WEIGHTED AVERAGE

Before jumping into quantum mechanics & Expectation values, let's discuss a few things on which these concepts are based. The term average is somewhat familiar to everyone, but the term weighted average is not so popular in general. To understand what these two terms mean, consider an example given below.

Suppose there are 3 people of mass 50 kg each and 1 person of mass 100 kg present in a room. Now, if someone asks, "What is the average mass in the room?" Then we may find out that,

$$\text{Avg. mass} = \overline{\text{m}} = \frac{100 + 50}{2} = 75 \text{ kg}$$

But this result is not so accurate. It ignores the fact that there are 3 people of mass 50 kg each. So here comes the concept of weighted average. The weighted average of the mass present inside the room is,

$$\text{Weighted Avg.} = \langle \text{m} \rangle = \frac{(3 \times 50) + (1 \times 100)}{3 + 1}$$
$$= \frac{150 + 100}{4} = 62.5 \text{ kg}$$

Now, this value shifts more towards 50 kg and is more accurate. So, a weighted average can reflect the importance of each component in a distribution. Hence its formal definition is, **"An average, resulting from the multiplication of each component by a factor reflecting its importance"** and in this example, importance reflecting factors of components 50 & 100 are 3 & 1 respectively. Usually, average values are denoted by $\overline{\text{A}}$ and weighted average values are denoted by $\langle \text{A} \rangle$.

III. WEIGHTED AVERAGE IN CLASSICAL MECHANICS

The concept of the **centre of mass** in classical mechanics is a nice example of how weighted average is applied to physical systems. To understand this, consider the simplest possible example given below.

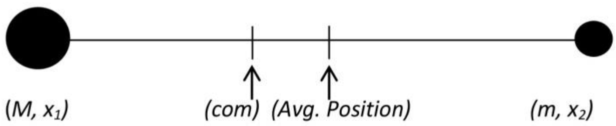

Figure 1. A system of two masses

Suppose there are two objects of masses M & m (M > m), lying on the x-axis of a frame of reference at positions x_1 & x_2 respectively, as shown in figure 1. In this system the average position of these two masses is, $x_{avg} = \frac{x_1+x_2}{2}$ & the **weighted average** position of these two masses is $x_{wtd.\ Avg} = \frac{Mx_1 + mx_2}{M+m}$. But this expression looks quite familiar. This is also the expression for the centre of mass of two objects. So, in classical mechanics, the centre of mass is nothing but the weighted average of different positions with different masses in a system and in this example the masses M & m are the important reflecting factors of positions x_1 & x_2 respectively.

IV. EXPECTATION VALUE IN DETAILS

To understand expectation values in detail, consider the following simple experiment. Let's consider a particle, whose motion is confined to the X-axis of a frame of reference and such a particle can be described by a wave function $\Psi(x, t)$. We can locate the particle, by measuring its position coordinate *'x'* and so, we have to produce a large number of these observations to find its average location more accurately. Now to do this, let's take N number of quantum mechanical systems containing a particle with the same state function Ψ.

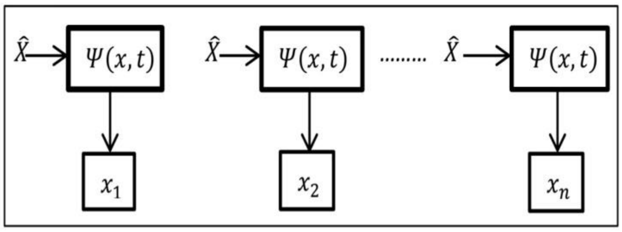

Figure 2. N number of Quantum Mechanical systems containing particles of the same state Ψ

Then try to locate the position of the particles in each system. Suppose the obtained positions of the particle are $x_1, x_{2,} x_{3,........} x_n$ and now we have obtained a large number of values of x. The average of all these measured values of positions in the state $\Psi(x, t)$ is called the expectation value of position operator $\hat{X}$, in the state $\Psi(x, t)$. But taking the ordinary average of these values is not going to work in this case. Because there is some probability (importance) associated with each value of x_n and here arises the concept of weighted average again. **In this case, the importance of reflecting factors are not just some random numbers or mass, they are probability. This means there is some definite probability of getting a position x_n in this experiment.** The probability of getting a position can be obtained from Born's interpretation [2] of wave functions and from his interpretations it is known that,

$|\boldsymbol{\Psi}(\boldsymbol{x_n}, \boldsymbol{t})|^2 \Delta \boldsymbol{x_n}$ = **Probability of finding a particle between $\boldsymbol{x_n}$ to $\boldsymbol{x_n} + \Delta \boldsymbol{x_n}$**

This is the **importance reflecting factor** of our experiment and now to get the weighted average of observed positions of the particle, we can write

$$\langle x \rangle = \frac{x_1|\Psi(x_1, t)|^2 \Delta x_1 + x_2|\Psi(x_2, t)|^2 \Delta x_2 + \dots\dots\dots\dots\dots + x_n|\Psi(x_n, t)|^2 \Delta x_n}{|\Psi(x_1, t)|^2 \Delta x_1 + |\Psi(x_2, t)|^2 \Delta x_2 + \dots\dots\dots\dots\dots + |\Psi(x_n, t)|^2 \Delta x_n}$$

$$or, \qquad \langle x \rangle = \frac{\sum_n x_n |\Psi(x_n, t)|^2 \Delta x_n}{\sum_n |\Psi(x_n, t)|^2 \Delta x_n}$$

For a very large number of observations (n→ ∞) the summation changes to an integral, i.e.

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} x|\Psi(x, t)|^2\, dx}{\int_{-\infty}^{+\infty} |\Psi(x, t)|^2\, dx} \qquad (3)$$

In terms of operators,

$$\langle \hat{X} \rangle = \frac{\int \Psi(x, t)^* \ \hat{X}\ \Psi(x, t)\, dx}{\int \Psi(x, t)^*\ \Psi(x, t)\, dx} \qquad (4)$$

$(\because \hat{X} = x\ , in\ position\ space)$

This is the same equation as equation (1) but in 1 dimension. Here finishes a formal derivation for the expectation value of the position. Similarly, we can derive an expression for momentum operator in momentum space [3] or any operator in general i.e.,

$$\langle \hat{P} \rangle = \frac{\int \Psi(p, t)^* \ \hat{P}\ \Psi(p, t)\, dp}{\int \Psi(p, t)^*\ \Psi(p, t)\, dp} \qquad (5)$$

$\left(\because\ \hat{P} = p\ , in\ momentum\ space\right)$

Now, it is clear that the expectation values in quantum mechanics are nothing but the weighted average of some observed values and the importance reflecting factors are just some numbers, which signifies the probability of getting a particular observed value. Furthermore, as we have discussed in the previous section, in classical mechanics, the concept of centre of mass is also based on the concept of weighted average and the importance reflecting factors are some masses in a particular position. So, we can say that the concept expectation value of an observable in quantum mechanics is analogical to the concept centre of mass of a system in classical mechanics. This means they are in two different branches of physics but their underlying mathematics is the same. Here finishes the conceptual development of expectation values and their relation with the centre of mass. Now let's discuss why it is called so. Means, why the name "expectation value".

V. REASON BEHIND THE NAME "EXPECTATION VALUE"

From classical mechanics, one may be familiar with the idea that the centre of mass of a system can be a point, where there is no mass at all and similarly expectation value of an observable can be a value, which may have nearly no probability of occurring at all. Then how can we call such a value an expected value? Let's see a problem for a better understanding of the situation.

Consider a hypothetical particle having a state given by the wave function,

$$\Psi(x) = \begin{cases} (1.01)\,(\sin x)^2\ , & -\pi \le x \le 0 \\ (\sin x)^2\ , & 0 \le x \le \pi \\ 0\ , & elsewhere \end{cases}$$

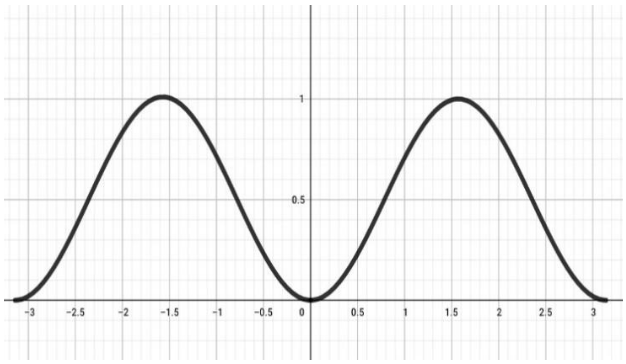

Figure 3. Graphical representation of the function $\boldsymbol{\Psi(x)}$

Its position expectation is,

$$\langle \widehat{\boldsymbol{X}} \rangle = \frac{\int_{-\infty}^{+\infty} \boldsymbol{\Psi(x\,,t)^*\ \widehat{X}\ \Psi(x\,,t)\ dx}}{\int_{-\infty}^{+\infty} \boldsymbol{\Psi(x\,,t)^*\ \Psi(x\,,t)\ dx}}$$

$$\langle\, \widehat{\boldsymbol{X}} \rangle = \frac{\int_{-\pi}^{0} \mathrm{x}(1.01)^2(\sin \mathrm{x})^4\, \mathrm{dx} \;+\; \int_{0}^{\pi} \mathrm{x}\,(\sin \mathrm{x})^4\, \mathrm{dx}}{\int_{-\pi}^{0} (1.01)^2\,(\sin \mathrm{x})^4\, \mathrm{dx} \;+\; \int_{0}^{\pi} (\sin \mathrm{x})^4\, \mathrm{dx}}$$

After evaluating the integrals,

$$\langle\, \widehat{\boldsymbol{X}} \rangle = \frac{-1.8877\ + 1.8506}{1.2017\ +\ 1.1781} = \frac{-0.0371}{2.3798} = -0.01558$$

From this result, it is clear that the expected position of the particle is around the origin. But what about its probability of being there? This question can be answered by looking at the graph of $|\boldsymbol{\Psi(x)}|^{2}$. Because from Born's interpretation, we know that $|\boldsymbol{\Psi(x)}|^{2}$ represents the ***probability density*** in space and by looking at its graph one can infer the probabilities at different positions in space. Here is the graph of $|\boldsymbol{\Psi(x)}|^{2}$ shown below in figure 4. From the graph, we can easily interpret that the probability of finding the particle is nearly zero around the origin and it's clear that expectation values are not the most probable values of a measurement and they may have a zero probability of occurring with zero expectations. So how to justify their name? The answer is, the concept of expectation value did not invent for use in quantum mechanics first. And it is important to note that most of the terminologies used in quantum mechanics were already there before the invention of quantum mechanics. The term "Expectation Value" had been already been there in the literature of probability theory at least 100 years before the invention of quantum mechanics. Particularly in gambling, the expectation value is a very well used term. For example, if one throws a dice and gain 2 Rupees when an odd number turns and lose 1 Rupee when an even number turn up and if one wants to guess in the long term with these rules what gain or loss to be expected, one has to calculate the "Expected value", which is nothing but a weighted average.

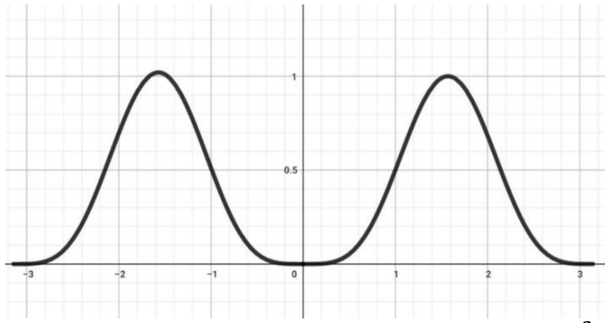

Figure 4. Graphical representation of the function $|\boldsymbol{\Psi(x)}|^{2}$

Therefore, the term expectation value is taken from probability theory. The centre of mass is also a weighted average, so one can call it also some expected value, but no probability is involved in the centre of mass so people avoid using the word expectation value.

VI. CONCLUSION

So far, we have discussed the concept of expectation values in quantum mechanics and its relation with the centre of mass in classical mechanics and we found that they are sort of **weighted average** of a given distribution. And the term **expectation value** is completely a probability theory creation and has nothing to do with quantum mechanics. In statistics at the fundamental level to characterize any statistical distribution one uses the terms **first moment**, second moment etc. The first moment of a given statistical distribution is also a kind of weighted average. In that sense, the expectation value and the centre of mass both are the first moments of some distribution. So, we can call them by whatever name we want. We can call them expectation values, weighted averages or first moments. One may also call the "expectation value" in quantum mechanics as **Centre of Probability** similar to the name **Centre of Mass**. So, at the end of the day, it's just a matter of convention to name, a concept in physics and everyone should feel free to understand things in their own way.

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