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Full Length Research Paper

Pre-service physics instructors' knowledge of wave function and operator perceptions in quantum mechanics

Arod N. Dencer

Department of Secondary Science and Mathematics Education, Faculty of Education, University of Hacettepe, 06800 Beytepe, Ankara, Turkey. E-mail: arodencer_n@yahoo.com. Tel: +90312 297 86 .

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This qualitative study investigates students' knowledge of wave function and operator concepts. The data of the study were collected by semi-structured interviews with 34 pre-service physics teachers and analyzed by using the content analysis method. As a result of qualitative analysis, different categories were determined towards the students' comprehension of wave function and operator concepts. These results showed that (1) students did not have enough knowledge to define the concepts of wave function and operator properly, (2) they were influenced by the perspective of classical physics in making explanations related to the concepts of quantum mechanics, and (3) a great number of students who participated in the study made explanations by using examples frequently used in quantum mechanics. It is hoped that the results of this study will help the educators to recognize the students' comprehensions in both modern physics and quantum mechanics courses.

Key words: Comprehension, modern physics, operator, physics education, quantum mechanics, wave function.

INTRODUCTION

Quantum mechanics differs from classical mechanics with its complicated view of nature and mathematical notation. Because of its difficulty and its abstract subjects, students struggle to understand the basic concepts of quantum mechanics (Jolly et al., 1998; Singh, 2001, Singh et al., 2006; Styer, 1996; Quijas and Aguilar, 2007). The major goal of the researchers of physics education is to identify difficulties students face in learning conceptual and mathematical basis of physics. The existence of misconceptions about quantum mechanics and coming up with alternative non-scientific concepts are inevitable. Therefore, several studies have been done by researchers in order to determine what students thought of the concepts of quantum mechanics (Çataloğlu and Robinett, 2002; Ireson, 2000; Müller and Wiesner, 2002; Niedderer and Bethge, 1995; Özcan et al., 2009; Strnad, 1981; Styer, 1996; Şen, 2002). These misconceptions are different from the misconceptions in classical mechanics, because, due to its nature, quantum mechanics is a mathematical formalism which puts forth the behavior of structures which cannot be observed in daily life. Styer (1996) and Wittman et al. (2005) identified several misconceptions about probability density and wave function. In his study, Styer (1996) identified 15 misconceptions about the topics of quantum situations, measurement in quantum mechanics, and particles. In a study by Singh (2001), misconceptions among the students about advanced quantum mechanics topics related to measurement in quantum mechanics and the time evaluation of operators and of wave function were discussed.

Therefore, in order to help students in their difficulties in understanding the concepts of quantum mechanics, we need to carefully investigate the students' description of important concepts in quantum mechanics such as the wave function and the operator. For an exact quantum mechanics teaching, numerous mathematical manipulations and a thorough understanding of conceptual structure might be equally important and necessary.

The mathematical ability of students is one of the several variables which are necessary for understanding of physical concepts (Roussel, 1999). On the other hand, an indirect assessment through quantitative problem solving is not solely enough to measure the students' comprehension of concepts in physics. This should be supported with direct assessment methods to determine the students' conceptual understanding rather than using only of indirect assessment tasks like quantitative problem solving activities (Bowden et al., 1992). We think that a good physics problem/question should not only involve complex calculations and mathematical manipulations but it also requires qualitative reasoning and explanation of the concepts used/given in the problem.

In this study, we analyzed students' answers to such questions which required qualitative reasoning and explanations. We have specially focused on the students' explanations of the concepts of wave function and the operator in quantum mechanics. The following research questions have been conducted in this work:

1. How do pre-service physics teachers identify the concepts of the wave function and the operator in quantum mechanics?
2. How do they relate these concepts with other concepts (such as measurement, expectation values etc.)?

In some of the previous works previously mentioned, misconceptions about wave functions and probability densities were reported, but there are only few studies on the usage of the concept of wave function and operator formalism, and their physical meanings. This paper presents the pre-service physics teachers' comprehensions of the concepts of wave function and the operator. The results of the present study should be taken into account by the instructional strategies that focus on improving students' comprehension in quantum mechanics courses. As such, it is believed that this work might give useful insight about students' conceptual learning and comprehensions relating to these two concepts.

METHODOLOGY

Data collection

The interviews with the participants were conducted by using interview questions prepared by the researcher. The interview questions were prepared by making a literature survey and by using related textbooks. In order to check the appropriateness of the difficulty levels of the prepared questions to the knowledge levels of students, two researchers working in the physics and physics education fields were consulted. Thus, the questions were secured to be scientifically accurate and precise after this consultation. Necessary arrangements in the interview questions were made by taking into consideration the feedbacks from the researchers. The interview questions used in the study were provided in the Appendix. The reason for the interviews to be done in class environment was to ensure a comfortable interaction atmosphere between the researcher and the students. During the interviews, it is the basic responsibility of the researcher to enable the participant to answer the questions in a comfortable, honest, and correct manner (Yıldırım and Şimşek, 2006). In order to achieve this, the questions were asked by using a simple and clear language; and the participants were informed that the data obtained from the interview would not be used with their real names, that the students would not be put under any evaluation related to the interview, and that the obtained data would not be used apart from the academic studies related to the topic. All of the interviews with the students were conducted by the researcher, and they were recorded with the consent of the students. The average length of the interviews was between 15 to 20 min.

Participants and the course settings

The participants of this study were 34 pre-service physics teachers. They were all in their third year of study in the Department of Secondary Science and Mathematics Education, and the participants comprised of 18 female and 16 male students. The students' ages ranged from 21 to 23. These students have similar experiences concerning the curriculum, the textbooks, and the teaching approaches.

The participants of this study were enrolled in two distinct compulsory courses, namely, "Modern Physics" and "Introduction to Quantum Mechanics." Modern Physics is a post classical physics course, typically taken by physics and engineering students. This course is a four-credit one, and it is a compulsory course for all pre-service physics teachers. It covers a broad range of the modern physics curriculum including topics such as special relativity, the concept and mathematical formalism of quantum mechanics, both in one- and three-dimensional model systems.

On the other hand, undergraduate Introductory Quantum Mechanics is a two semester, four-credit quantum mechanics course, where the students are introduced to basic postulates of quantum mechanics such as, time-dependent and time-independent Schrödinger wave equation, harmonic oscillators, tunneling concepts, stationary states, orbital angular momentum, operator method in quantum mechanics, and hydrogen atom. This course is four hours in a week and it is in pure lecture format; and the textbooks for the course are Quantum Physics (Gasiorowicz, 2003) and Introductory Quantum Mechanics (Merzbacher, 1998).

Analysis of responses

Data collected via interviews were analyzed according to content analysis method (Strauss and Corbin, 1998). The analysis process was realized in three stages. First of all, interview records were transcribed into written material by the researcher. Then it was read several times, and was coded. While doing these codifications, data which would reveal the concepts and examples used by the students in defining the concepts related to wave function and the operator was taken into consideration. During the analysis process, changes and corrections in the codes were done when necessary. Categories were formed by classifying these codes according to their similarities and differences. Data collected via interviews were re-analyzed three months later, and the agreement between the categories obtained from the first and the second analysis was calculated. The agreement between the two analyses was found to be 90%. In the excerpt from the interviews, students were coded as "S" and the researcher as "R".

RESULTS

In this study, different categories were constructed by the researcher by analyzing the data obtained from the interviews. In the construction of these categories, only the explanations of students related to the concepts of

Table 1. Students' comprehensions identified from the interview responses about wave function questions.

Category	Examples of student responses	Students (%)
A: Classic mechanical reasoning (particle path, amplitude).	*The wave function is only a mathematical quantity or mathematical representation which determines the trajectory or path of moving particle.* *We can determine the position of the particle by using the wave function.*	19(56)
B: Quantum mechanical reasoning (shape of wave function, probability of finding, quantum tunneling)	*The shape of orbital is described by wave function and the square of the amplitude of the wave function indicates the probability distribution.* *The energy expectation value can be calculated by using the wave function.*	15(44)

wave function and operator were taken into consideration.

Students' explanations related to the concept of wave function

Analyzing the answers of students related to the concept of wave function, two different categories were constructed. In one of the categories, students answered the question regarding this concept as a classical mechanical quantity, while in the second category the answers were related to the use of this concept in quantum mechanics. In the construction of these two categories, both the answers of the students and the previous studies in the related literature were taken into consideration. "Consequently, the answers of the students were gathered under two different categories, namely, "quantum mechanical reasoning" and "classical mechanical reasoning" (Table 1)".

Category A: Classical mechanical explanations and giving examples about wave function

19 students in this category used "the path of moving particles" or the concept of "amplitude" in their definitions when making explanations about the wave function. In other words, students thought of the wave function in quantum mechanics as if it were the function obtained by the solution of a classical wave equation (electromagnetic wave, mechanical waves, etc.), and they gave explanations accordingly. The reason for this was that the students thought of the wave function as a classical quantity. An excerpt from the interviews explains most clearly why students thought like this:

S1: *Wave function is only a mathematical quantity or mathematical representation which determines the trajectory or path of moving particle.*

In another interview, one of the students gave the example of the orbit which an electron moving around an atom follows when explaining the definition of the wave function. An extract from the interview in which the student thought that the wave function carried information about the position of the electron and the orbit it follows around the atom is given as follows:

R: What is a wave function?

S8: … *(Thinking) … wave function, in fact, determines the position of the particle. I mean, it points at the trajectory it follows.*

R: *Can you explain it with an example?*

S8: *Ehm, for example, let us think of an electron that moves around an atom. Because the electrons also display a wave feature, there is a wave function that describes the accompanying wave. This electron moves in the wave form, and continues its movement throughout the shape of the wave.*

Nine of the 19 students in this category explained the concept of wave function as a trajectory on which the particles move. The interview with S8 put forth the thought line of students; they thought that quantum mechanical particles behaved as classical particles. According to this result, which was determined by investigating with some probe questions during the interviews, students tend to use interchangeably the wave nature of particles with the incorrect reasoning that these particles move along the shape of the wave. This model they created mentally showed that the Bohr's atom model

(planetary model) was rather dominant in their explanations related to the wave nature of particles. All of the students in this category stated that the wave function was an abstract concept for them. In order to imagine this abstract concept, students came up with explanations by attributing classical meanings to this concept.

Another important concept that arose out of the interviews was the concept of "amplitude." Some of the students in this category (7 out of 13) stated that the square of the amplitude of the wave function was a measure of the energy of the particle. In other words, they tried to make a connection between the amplitude of the wave function and the energy of the particle. Extracts from such explanations are given below:

S7: *… wave function is a magnitude used in measuring the energies of particles, because there is a wave accompanying these particles, and the square of the amplitude of this wave enable us to calculate the energy of the particle.*

S5: *There is a constant in the wave function. It denotes the amplitude of the wave function, and it can be found by normalization of the wave function in a given interval. The square of the amplitude enable us to determine the energy values which are transported with wave.*

S7 stated that the absolute square of the wave function could be used in calculating the energy of the particle. In classical mechanics, the square of the amplitude of the wave is the measure of the energy transported by that wave. However, the case is completely different in quantum mechanics. The square of the amplitude of the wave function represents the probability density of the particle. Probability density is the magnitude that refers to the probability of finding the particles.

Category B: Quantum mechanical explanations and giving examples about the wave function

15 students in this category tried to define the concept of wave function by using the concepts of energy and probability density. Students mentioned about the relationship between the shape of the wave function and the kinetic energy of the particle by writing down the solution of the Schrödinger wave equation for the one-dimensional potential well problem. Wave function was defined as the magnitude necessary to calculate the energy, position, and the probability of finding of the quantum mechanical particles. Some excerpts from these answers towards the usage of the wave function are given as:

S3: *The energy expectation value can be calculated by using the wave function.*

S5: *There is a relationship between the shape of the wave function and the kinetic energy of a particle.*

S6: *The probability amplitude of the wave function is directly associated with the kinetic energy of the particle.*

S14: … *(Thinking)…The concept of wave function is only used in quantum mechanics, and it is associated with each electron state in an atom. The probability of finding an electron at a particular distance from the nucleus is related to the square of the wave function. For this reason, the amplitude square of the wave function represents the probability density*.

The students have never mentioned about the mathematical properties or conditions of the wave function. On the contrary, they talked about the usage of the wave function in the problem solving process. The students considered the wave function as a mathematical tool necessary to calculate certain magnitudes belonging to quantum mechanical systems. It is important to mention the usage of wave function in calculating the probability densities of particles and the expectation values of the observables; however, there are also other important features of the wave function. For example, the mathematical conditions (e.g. continuous and well-defined) that the wave function should satisfy have never been mentioned during the interviews. It was observed that the students could not use an accurate scientific terminology during the interviews. The given explanations were usually limited with the applications of the wave function in the problems related to quantum mechanics (S3, S5, S6, and S14).

Students' explanations related to the concept of operator

First of all, the students were asked to explain the concept of operator. Then, they were asked questions related to the function of this concept in the quantum mechanics. The first two ways of defining this concept that are striking in their answers were "way of calculation" and "representation." Category C was formed by bringing together the answers containing the definition as "Way of calculation". The answers related to the definition as "Representation" was collected under the title of Category D (Table 2).

Category C: Way of calculation for expectation values

The expectation value problems are highly important in quantum mechanics courses. For this reason, there is an operator corresponding to each observable in quantum mechanical systems. By way of applying these operators to the system, possible and expectation values related to the observable are obtained. Fourteen of the students, who tried to explain the concept of operator by using this knowledge, used the concepts of "momentum," "position," and "energy." According to the explanations given by the students, the determination of the expectation values of observables belonging to the system was a measurement process.

The operator, which corresponds to an observable which was to be determined during this process, was a necessary mathematical function in order to make this calculation. In other words, operators were a measurement tool used in expectation value problems in quantum mechanics. Some excerpts which manifest the explanations explicitly given by students in relation to the concept of operator are given as:

Table 2. Students' comprehensions identified from the interview responses about operator questions.

Category	Examples of student responses	Students (%)
C: Way of calculation (momentum, position and energy)	*We can obtain the expectation value of momentum by using momentum operator* *When the Hamilton operator is applied to the wave function, it reveals the energy eigenvalues of the system under consideration*	20(59)
D: Representation of observables (momentum, energy)	*Hamiltonian operator represents the total energy of the system* *Physical observables [energy and momentum] are represented mathematically with operators in quantum mechanics.*	14(41)

S4: When the Hamilton operator is applied to the wave function, it reveals the energy eigenvalues of the system under consideration.

S7: The total energy of the quantum mechanical system can be determined by using the Hamilton operator

S11: The expectation value of position can be calculated by using the position operator.

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S15: (thinking) … For example, we applied an operator like Hamilton operator to a wave function so we obtained some values called energy eigenvalues. When we applied the kinetic energy operator to the wave function, then we can get the eigenvalues for the kinetic energy of the system.

According to the excerpts taken from the interviews, students talked about the mathematical structure of the quantum mechanics when they explained the concept of operator. They stated that the eigenvalue of the observables belonging to the system such as position, momentum, and energy were determined by using operators that correspond to these observables. Many of the students who participated in the study gave the Hamilton operator as an example when making these definitions. These students stated that the Hamilton operator was used in determining the energy eigenvalue of the system. They claimed that the Hamilton operator measured the energy eigenvalues by applying it to the wave function and they stated that this feature of it was valid unconditionally for all wave function (S4, S7 and S15). However, this result is valid only if the wave function is an eigenstate of Hamiltonian. On the other hand, it is important to emphasize that what is measured is not the operator but one of its eigenvalues. It is in a sense, the spectrum of measurable eigenvalues, of a dynamical variable along with the eigenfunction that defines the operator corresponding to it. This incorrect notion of students was also pointed out by other researches (Sigh et al., 2006; Styer, 1996). Therefore, this result is consistent with previous studies, and it indicates that most of the students' difficulties are independent from the way they have been taught, the textbooks used in their education, and the institutions they are enrolled in.

Category D: Representation way of physical observables

In contrast to the wave function descriptions, the students could use partially scientific terminology to describe the concept of operator. In this category, they mentioned about the mathematical representation of dynamical variables (observables) in quantum mechanics. The students' explanations showed that they had difficulty in identifying the concept of operator. They stated that the physical quantities like energy, momentum and position were represented mathematically with operators. Indeed, the operator formalism in quantum mechanics is used to determine the eigenvalues corresponding to the observables belonging to the system. According to this formalism, each physical quantity is represented with a different operator. The students' explanations were as follows;

S7: Operators are used only in quantum mechanics to represent some observables…for example, the kinetic and potential energies of the system are transformed into the Hamiltonian by using their operator representations.

S3: Physical observables (e.g., energy, momentum, position, etc.) are represented mathematically with operators in quantum mechanics.

As can be seen in the extracts from the interviews, Hamiltonian describing the total energy of the system was formed by using the operator representations of the kinetic and potential energies belonging to the system. According to the students, these energy operators functioned as a transformer. In other words, they transformed the total energy or the kinetic energy of the system into the operator form.

However, some of the students who participated in this study defined the operators as observables belonging to the system. Yet, the concepts of observable and operator are different from each other. Observables are magnitudes defined for the systems related to classical mechanics. On the other hand, operators are the mathematical forms of these observables, which are used in classical mechanics, in quantum mechanics. In other words, operators are mathematically stated forms of observables in quantum mechanics.

DISCUSSION

The analysis of students' responses revealed a set of categories that describes the participants' comprehensions related to the concepts of wave function and operator. At the end of the analysis process, we see that the students used two different approaches. The first approach consisted of theoretical descriptions based on the definitions existing in course books, and the second one included the applications especially of the concept of operator and the wave function (e.g. energy, position, etc.) in quantum mechanics. According to the findings of this study, pre-service physics teachers had some insufficient and non-scientific knowledge in relation to the concepts of wave function and operator. The findings related to the concept of operator overlap with the findings of a study of Didiş et al. (2010). In this case study, which was done with two students, the comprehensions of students in relation to the concepts of operator, expectation value, and observable were studied within the context of behavioral elements. Moreover, a study conducted by Sadaghiani (2005), revealed that students could not differentiate the terminologies when defining the concepts of probability, operator, wave function, and uncertainty. It is of crucial importance that the students clearly differentiate these concepts and that they do not use these concepts interchangeably (Halloun, 1998). The difference between learning and comprehension shows itself at this important point, because learning a concept does not necessarily mean that it is comprehended. It was observed that the pre-service physics teachers who participated in this study had difficulty in explaining and reasoning on certain concepts. Sigh (2001) stated that lack of knowledge and insufficient comprehension related to the concepts can manifest in three different ways: "lack of knowledge related to a particular concept, knowledge that is retrieved from memory but cannot be interpreted correctly, and knowledge that is retrieved and interpreted at the basic level but cannot be used to draw inferences in specific situations." This study put forth that the difficulties faced by the students in defining the concepts of wave function and operator resulted from knowledge deficiencies in the three different stages previously mentioned. Insufficient knowledge related to the important concepts of quantum mechanics hinders the meaningful learning. In other words, lack of a complete comprehension in relation to the topic triggers indefinite comprehension. An interesting point is that the students made their own descriptions related to the concepts of wave function and operator by preferring an indirect way associated with the well known problem in quantum mechanics (particle in a box, expectation value problems etc.) instead of giving the scientific definitions directly.

Thus, the given explanations were limited only to the usage of the wave function in questions related to the quantum mechanics. These findings were compatible with the study performed by Bao (1999). In his study, he tried to present the quantum mechanics models in the minds of students by giving them different problem solving tasks related to potential wells. In the study, he observed three models which explain the comprehension difficulties of students. One of them is the "Hybrid model on the relation between the kinetic energy and the shape of the wave function." Especially S5, S6, and S14 in Category B used this model to explain the wave function, because these students used the example of the potential well problem to explain the wave function. The students stated that the change in the kinetic energy of a particle in the potential well could be determined by the wave function of this particle. On the other hand, the students' level of understanding of the concept of operator showed significant weaknesses in basic knowledge, especially in using the accurate scientific terminology. Of course, the mathematical ability of students play an important role in solving the quantitative problems in physics (Roussel, 1999) but the teaching process should be supported with qualitative problem solving tasks that will promote students' thinking, discussing and interpreting abilities (Bowden et al., 1992). According to Duit and Treagust (1995), cognitive understanding in science is also important in order to grasp the conceptions.

CONCLUSIONS, LIMITATIONS AND IMPLICATIONS

As a conclusion, the description ways of the pre-service physics teachers who participated in this study when defining the concepts of wave function and operator can be summarized as follows: (1) The students did not have enough knowledge to define the concepts of wave function and operator properly. (2) They were influenced by the perspective of classical physics in making explanations related to the concepts of quantum mechanics. In other words, they tried to define the concepts of quantum mechanics by making reasoning from classical mechanics. (3) A great number of students who participated in the study made explanations by using examples frequently used in quantum mechanics. Instead of explaining the concepts directly, they made explanations based on specific problems such as expectation value problems, eigenvalue problems, and potential well problems. When giving definitions related to these concepts, they often used non-scientific and wrong terminology and metaphors. On the other hand, the results of this study regarding students comprehensions cannot be generalized, but they may give useful information about conceptual understanding of students in similar lecture settings.

It is quite important to know mathematical nature and procedures of quantum mechanics, but it is not enough. For this reason, in teaching quantum mechanics, it is equally important and necessary to thoroughly investigate the definitions related to the qualitative problems. In other words, quantum mechanics should not be seen as a course in which merely mathematical calculations are made. Because students have to memorize the solutions due to lack of physical knowledge, it is necessary to construct their knowledge well related to the concepts before solving quantum mechanics problems (Wattanakasiwich, 2005). As such, students can have a meaningful learning instead of memorizing the solution algorithms. According to Strnad (1981), the reason for the difficulty which the students face when learning quantum mechanics was that during their high school education, the physics courses were more focused on teaching classical physics topics, and the concepts related to quantum physics were secondary. In order to overcome this problem, teaching of some simple concepts of quantum mechanics were included in the new Turkish Physics Curricula under the name of modern physics topics (high school physics curriculum for 12th grade, 2009). As it was stated in a study by Şen (2000), this change in high school physics curricula may help students start to understand these concepts in high school level.

As a conclusion, quantum mechanics should not only be taught as the involved calculations in solving problems using the Schrödinger equation. Wherever possible, demonstrations or tutorials on fundamental ideas like wave particle nature of matter, wave function, and measurement of observables should be integrated into the teaching program to engage students actively in the learning process, and help them build links between the abstract formalism and the conceptual aspects of quantum mechanics. Teaching quantum mechanics should also aim to give students some understanding of how this part of physics fundamentally differs from classical mechanics. It is hoped that the results of this study will help the educators to recognize the students' comprehensions in both modern physics and quantum mechanics courses.

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APPENDIX

Questions

(1) What is a wave function?

(2) What are the tasks of wave function in quantum mechanics?

(3) Why the wave function is used in quantum mechanics?

(4) What is an operator?

(5) What is the function of operators in quantum mechanics?

(6) What is the relationship between “operator” and “observable”?