STUDENTS’ CONCEPTUAL DIFFICULTIES IN QUANTUM MECHANICS: POTENTIAL WELL PROBLEMS

ÖZGÜR ÖZCAN*, NILÜFER DIĞİŞ**, MEHMET FATIH TAŞAR***

ABSTRACT: In this study, students’ conceptual difficulties about some basic concepts in quantum mechanics like one-dimensional potential well problems and probability density of tunneling particles were identified. For this aim, a multiple choice instrument named Quantum Mechanics Conceptual Test has been developed by one of the researchers of this study and administered to 95 upper-class undergraduates and 15 graduate level students at physics education and physics departments at three universities in Turkey. In addition, in order to be able to gather more information about how students understand these concepts, semi-structured interviews were conducted with selected five undergraduate and five graduate students. Common student difficulties which are deemed to stem from thinking based on classical mechanics were determined. These difficulties should be taken into account by instructional strategies that focus on improving student understanding of potential well problems and quantum tunneling concepts.

Keywords: Conceptual test development, potential well problems, probability density, tunneling effect, quantum mechanics


Anahtar sözcükler: Kavramsal test geliştirme, potansiyel kuyu problemleri, olasılık yoğunluğu, tünel olası, kuantum mekaniği

1. INTRODUCTION

Quantum theory is a successful theory of physics which describes, correlates and predicts the behavior of (Merzbacher, 1998) subatomic systems. It caused fundamental changes (a paradigm shift) in human ideas concerning the laws of the nature and subsequently leads to immense technological revolutions. However, for the most, conceptually understanding of the fundamentals of the new paradigm has not been any easier.

One of the major goals of physics education researchers is to identify student difficulties in learning conceptual and mathematical basis of physics. For undergraduate level physics students, it seems more difficult to learn concepts of the quantum theory because of many reasons such as the probabilistic approach for determining the position of a particle, uncertainty relations between observables, non-physical abstract wave function which carries all information about particle, collapse of wave function, and usage of advanced mathematics and different notations. However, learning of the quantum mechanical concepts are important (Penrose, 1989), since it provides scientists the ability to make calculations and conduct experiments and thereafter to create new technologies based on the behavior of atomic scale objects (Faye, 2002).

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The purpose of this study was to determine students’ conceptual difficulties in quantum mechanics by focusing on one-dimensional potential well problems and the probability density of tunneling particles.

2. LITERATURE REVIEW

Quantum mechanics differs from classical mechanics in many characteristics. One of the obvious differences is its complicated mathematical notation. Strnad (1981) explained that learning difficulties at high school level stem from the fact that there was an over emphasis on classical physics which leaves little or no space for teaching quantum concepts. On top of that students are not adequately trained to meet the necessary mathematical pre-requisites. For an effective learning of quantum mechanics, numerous mathematical manipulations and deep understanding of the conceptual structure are equally important and inevitable.

While trying to understand the abstract concepts from their definitions, misconceptions are unavoidable for quantum mechanics. Physics education research groups study for the same aim to provide conceptual learning of all branches of physics. For this reason, researchers tried to understand students’ conceptions in quantum mechanics (Çataloğlu, 2002; Ireson, 2000; Müller & Wiesner, 2002; Niedderer & Bethge, 1995; Styer, 1996; Wittmann, Morgan, & Bao, 2005). Common misconceptions of quantum mechanics differ from misconceptions in classical mechanics, since, visualizations of its concepts are almost impossible in daily life. In quantum mechanics, some misconceptions such as quantum states, measurement, identical particles and some other concepts are more frequently encountered as compared to others. Styer (1996) and Wittmann et al. (2005) reported some misconceptions about wavefunctions and probability densities. Moreover, our macroscopic world is well explained by classical theories while quantum theory describes the relationships between microscopic quantities. Some researchers reported that the students’ mathematics scores correlated highly with their physics scores (Hadzidaki, Kalkanis, & Stavrou, 2000). On the other hand, Roussel (1999) explained that the mathematical ability was one of the several variables which were necessary for understanding physical concepts. However, taking and passing typical introductory mechanics and calculus courses are not sufficient indicators of conceptual understanding of physics for college students. Students may show misconceptions even after taking courses and graduating from universities. In the literature there are also some studies that showed that students do not possess well defined mental models about tunneling of the particles (Morgan, Wittmann, & Thompson, 2004; Redish, Wittmann, & Steinberg, 2000; Wittmann & Morgan, 2004).

3. QUANTUM MECHANICAL BACKGROUND

The concept of potential energy diagrams has great importance in quantum theory (Jolly, Zollman, Rebello, & Dimitrova, 1998). Because of insufficient energy of the particles to overcome the barrier, they can never appear at x>a classically which is not the case in the quantum realm, i.e. particles can penetrate through the barrier. This situation is called quantum mechanical tunneling. Classically, particles can never be observed in the forbidden region (0 < x < a) where the ‘a’ is barrier width, however in quantum mechanics they can tunnel through that region and they can be observed at x>a (Krane, 1996, p.164).

Sometimes, the tunneling effect of a particle can not be considered as a physical event since students can not find any actual corresponding event to consider. In quantum mechanics lectures, the example of alpha decay (escape of alpha particle from nucleus) (Krane, 1996, p.164) should be given as a physical example during learning the tunneling concepts. Also the working principles of tunnel diode and scanning tunneling microscope (Krane, 1996, p.164) should be mentioned in quantum mechanics courses.
4. METHODOLOGY

4.1. Data Collection

This study is composed of two parts: development and application of a conceptual test and conducting semi-structured interviews with selected students. During the development of the instrument, firstly a questionnaire with five open-ended questions covering the basic properties of quantum mechanics concepts was administered to identify students’ level of knowledge. Each of the questions in the final test was prepared by considering the students’ common difficulties which were identified with the open-ended questions. For some of the items students were asked to provide extended responses. The Quantum Mechanics Conceptual Test (QMCT) was developed in the light of these data. The test was examined and evaluated by three physics professors in order to establish the content and construct related evidences for the validity of test results. Moreover, the consistency of mathematical, verbal and visual elements of the test was examined by experts. In the pilot study, this test was administered to 80 students. And some items were excluded by consulting faculty members from the departments of physics and physics education. The reliability coefficient \( \alpha \) of the multiple choice test was calculated to be .79 which is considered good by the standards of test designs (Nitko, 1996) and the point bi-serial discrimination coefficients were determined to be between 0.3 and 0.8 for all questions.

For the second part of the study a total of 10 participants were selected purposefully according to their test results for semi-structured interviews (Maxwell, 1996, p.70). For the aim of obtaining more detailed and accurate information and determining the difficulties about participants’ reasoning the students who answered some questions correctly but explained their reasoning incorrectly were also selected in this group.

The possibility of reliably administration to large samples in a short period of time and the easy data analysis procedures may be cited as an advantage of using objective type item tests. Also, objective type item tests may indicate the general tendency of large numbers of students about concepts. However, in order to get detailed information about students’ reasoning, interviewing is a good data collection method.

4.2. Participants of the Study

Final form of QMCT contains 20 questions. It was administrated to 95 upper-class undergraduate and 15 graduate students in physics education and physics departments of three universities. Ten interviewees (five undergraduate and five graduate students) were selected in this sample and semi-structured interviews were conducted.

4.3. Data Analysis

Both quantitative and qualitative data were collected and analyzed. The descriptive statistics were done by using Statistical Package for the Social Sciences (SPSS) and the qualitative data (open-ended questions and the translation of the student interviews) were analyzed by the researchers both individually and collectively.

5. FINDINGS

The purpose of this study was to investigate the students’ understanding of basic concepts of quantum mechanics including one-dimensional potential well problems and probability density of tunneling particles. Below interview excerpts are given in order to illustrate student’s level of understanding of what a potential well is and their conceptual difficulty on this concept.

One of the 4th grade level pre-service physics teacher students who completed a quantum mechanics course defined the potential well problem after test administration as follows: 

**Student (S)**: Mmm… Potential well, there is a deep well, and there is a small particle in it. It cannot escape from there in classical mechanics, but it has a probability to escape from there in quantum mechanics.
**Interviewer (I):** Can you give an example for this situation?

**S:** For example... Mmm... Pull on an electron toward nucleus. There is such a potential, such a force... I think that it is impossible to break off a particle from there. The escape of a particle is very interesting.

The physics teacher candidate’s statements show that she thought a potential well as a “concrete well”. In addition, her explanations about the possibility of a particle’s escape are based on memorization (or low level understanding), since she has no clear explanations and specific examples of this situation. The findings suggest that this student’s difficulty is related to qualitative understanding. This result is similar to the one obtained by Singh, Belloni, and Christian (2006) which explained students’ difficulties as not being able to answer questions verbally to reflect conceptual understanding, although they could solve mathematical versions of the same problems.

One of the potential well questions from QMCT is shown in Figure 1 below.

![Diagram of a potential well](image)

**Which one of the followings is true for the tunneling of a particle with a total energy \( E < V_0 \)**

A) Total energy in region I is the same as the total energy in region II
B) Kinetic energy of the tunneling particle is the same in region I and in region II
C) Total energy in region I is less than the total energy in region II
D) Potential energy of the particle is decreased.

**Figure 1:** A barrier penetration question from the QMCT.

Results are given in Table 1 and in Table 2. The main intention in this item was to probe students’ ideas about the energy of a tunneling particle. In introductory quantum mechanics textbooks the solution of the Schrödinger equation in both regions are given and often the transmission coefficient and the wave function of the particle are discussed. However, students’ responses to this item, as seen in Table 1 and in Table 2, clearly show the most of the students (37 out of 95 undergraduate and six out of 15 graduate students) do not understand the energy concept (potential, kinetic and total) of the tunneling particle in different region very well. Most of the undergraduate students (58 out of 95 undergraduate students) selected the correct answer of the potential barrier question (see Figure 1). However, some of these students (13 out of 58 undergraduate students) had an incorrect reasoning about the energy loss of the tunneling particle. They stated that the wavelength of the tunneling particle has the same value in region I and in region II. Because of the same reason, 12 undergraduate students selected the incorrect answer which included the kinetic energy of the particle as same in region I and in region II. On the other hand, 25 out of 95 undergraduate students claimed that the particle must lose a part of its total energy to pass through the potential barrier. Moreover, several students have written expressions that can be paraphrased as “the particle should use some part...
of its potential energy therefore the kinetic energy of the particle must be constant during the tunneling process”.

Table 1: Distribution of Undergraduate Level Students’ Answers to the Energy of Tunneling Particle in Different Regions.

<table>
<thead>
<tr>
<th>Students’ Major</th>
<th>Total energy in region I is the same as the total energy in region II</th>
<th>Kinetic energy of the tunneling particle is the same in region I and in region II</th>
<th>Total energy in region I is less than the total energy in region II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physics (N=50)</td>
<td>( N ) 70 %</td>
<td>5 10 %</td>
<td>10 20 %</td>
</tr>
<tr>
<td>Physics Education (N=45)</td>
<td>23 51 %</td>
<td>7 16 %</td>
<td>15 33 %</td>
</tr>
<tr>
<td>Total (N=95)</td>
<td>58 61 %</td>
<td>12 13 %</td>
<td>25 26 %</td>
</tr>
</tbody>
</table>

Table 2: Distribution of Graduate Level Students’ Answers to the Energy of Tunneling Particle in Different Regions.

<table>
<thead>
<tr>
<th>Students’ Major</th>
<th>Total energy in region I is the same as the total energy in region II</th>
<th>Kinetic energy of the tunneling particle is the same in region I and in region II</th>
<th>Total energy in region I is less than the total energy in region II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physics (N=10)</td>
<td>( N ) 70 %</td>
<td>1 10 %</td>
<td>2 20 %</td>
</tr>
<tr>
<td>Physics Education (N=5)</td>
<td>2 40 %</td>
<td>2 40 %</td>
<td>1 20 %</td>
</tr>
<tr>
<td>Total (N=15)</td>
<td>9 60 %</td>
<td>3 20 %</td>
<td>3 20 %</td>
</tr>
</tbody>
</table>

Almost all of the interviewed students’ gave similar responses to each other for the energy of a tunneling particle. Each of the five undergraduate students mentioned that the energy was definitely lost during the tunneling process. A typical interview excerpt explaining this situation and taken from the interview with an undergraduate student is given below. This result is also similar with others obtained in earlier studies (Morgan et al., 2004; Redish et al., 2000).

I: What kind of an energy the particle has in region I (see Figure 1)
S3: Mmm… Kinetic energy…
I: Ok. How do you compare the total energy of the particle, in both regions?
S3: Mmm… In region II the total energy is less then in region I.
I: How do you explain this result?
S3: Mmm… the particle must spend a part of its kinetic energy to pass through the potential barrier. The particle has only kinetic energy in region I. Because of this reason, in region I the momentum of the particle is larger than in region II.

In this interview we probed the student’s thinking about what kind of energy is being lost in the tunneling process. According to the QMCT results (see Table 1 and Table 2) many students who thought the energy was lost, did not have a clear idea of which energy was being lost. By means of this interview we elicited the student’s idea about the relationship of potential, kinetic and total energy in the context of the tunneling. Other interviewed students (four of the five undergraduate students) mentioned that the potential energy is being lost during the tunneling of a quantum particle.
Another interview excerpt taken from an interview with graduate students was as follows:

I: As you see, the kinetic energy of the particle is less than the barrier potential in region I. Can this particle pass through this potential barrier?

S1: Sure… but if we think this process as quantum mechanical…

I: Ok. What do you mean with quantum mechanical, can you explain that further?

S1: Mmm…. In quantum mechanics there is a duality principle. The particles can behave sometimes as a particle and sometimes as a wave. Tunneling of a particle can only be explained with quantum mechanics, because quantum mechanics can describe the microscopic systems. The solution of the Schrödinger equation gives the transmission and reflection coefficients which cannot be obtained in classical physics.

I: What can you say about the wave function amplitude in both regions?

S1: Mmm…the amplitude of the wave function in region II is smaller than the amplitude in region I.

I: So then, what do you think about probability finding of the particle?

S1: Mmm… In region II the probability finding of the particle is less in region I.

I: Could you describe that a little bit further?

S1: Ok… Mmm…the kinetic energy of the particle is larger in region I. Because of this reason the momentum of the particle is larger than in region II.

In another item (item 17) in the test, we asked students to determine the correct wave function for a given linear potential well (see Figure 2). Here, the question aimed to probe the students’ knowledge of the relationship between the kinetic energy and the probability distribution of a moving particle in one-dimensional potential well and the graphs included the answer choices should be interpreted as follows:

**Graph I:** The probability density of the particle takes the biggest value in the middle of the potential well. Moreover, the wave function behavior must be symmetrically relative to the center of the potential well and the wavelength of the particle decreases when it moves towards the ends of the potential well.

**Graph II:** The students’ should know the relationship between the wave number and the kinetic energy of the particle. The larger kinetic energy in the right and left sides results in a larger number of waves. Moreover, in this graph the wavelength of a moving particle is constant with time.

**Graph III:** The probability density of the particle is zero in the middle of the potential well. Because of the smaller kinetic energy, the particle must spend more time around the middle of the potential well. The amplitude of the wave function must be larger than the left and right sides of the potential well, if this graph was the correct answer.

More than 50 % of the students in both departments failed to give the correct answer for this item (see Table 3). The most commonly given incorrect answer by graduate students of both departments was choice D. It now emerges as the distracter for this item. Although choice D is similar to the correct answer (choice A), it reflects a constant wavelength with time. This shows that these students did not consider decreasing wavelength of moving particle with increasing momentum with time. Five out of 10 graduate physics majors (50 %) selected choice D as their answers and 3 out of 5 graduate students in physics education departments (60 %) also selected this choice. Some students (20 %) in both departments chose answers that included constant wavelength (see choice C) showing their difficulty in understanding the concept of probability of the wave function. Another possible reason for students not selecting the correct answer of this item could be their poor understanding of the relationship between probability density and the momentum of the particle. In a follow-up interview some of the students argued that the smaller kinetic energy in the middle gives smaller amplitude to the wave function. This reasoning can be interpreted as resulting from students’ knowledge of the classical wave phenomena. This result constitutes another example of students using their classical knowledge for explaining quantum mechanical concepts. It is very ordinary for the
students to use the classical models to explain the quantum mechanical phenomena since they may not be familiar with or provided an appropriate quantum mechanical model.

The plot below shows potential energy function $V(x)$ versus $x$, of a symmetric infinite well. The infinite well is of width $2a$ and $V(x) = V_0 \frac{1}{a} (1+x/a)$, for $x$ between $(-a, 0)$ and $V(x) = V_0 \frac{1}{a} (1-x/a)$, for $x$ between $(0, a)$.

Which one(s) of the figures below is/are most likely to be a physically acceptable energy eigenstate solution(s) for the time-independent Schrödinger equation for this well?

A) Only I
B) Only II
C) Only III
D) I and III

Explain your choice:

![Potential Energy Function](image)

**Figure 2:** A linear potential well question from the QMCT.

**Table 3:** Distribution of Graduate Level Students’ Answers to the Probability Density of a Particle in a Given Linear Potential Well.

<table>
<thead>
<tr>
<th>Students’ Major</th>
<th>Distribution of the graduate students’ responses</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Only I</td>
</tr>
<tr>
<td></td>
<td>$N$</td>
</tr>
<tr>
<td>Physics (N=10)</td>
<td>2</td>
</tr>
<tr>
<td>Physics Education (N=5)</td>
<td>1</td>
</tr>
<tr>
<td>Total (N=15)</td>
<td>3</td>
</tr>
</tbody>
</table>
Only two of the interviewed graduate students were able to explain the correct reasoning for item 17. Below are the excerpts from those interviews.

S3: …I am not sure, but I think the probability amplitude of the wave function must decrease with time, while the kinetic energy of particle increasing...

S4: …the momentum of the particle takes the minimum value in the middle of the potential well. For this reason, the probability amplitude must take the biggest value...

We have determined similar incorrect results for this item (item 17) among undergraduate physics and physics education majors (see Table 4). Most of the students (39 out of 95 undergraduate students) picked the distracter (choice D). This shows that the students have many difficulties with associating the wave function with the kinetic energy of the particle which is moving in the given potential well. In interviews we encountered that the most of the students were not able to elucidate the qualitative reasoning based on time and momentum. On the other hand, some undergraduate students do not know the relation between the wave number and the kinetic energy of the particle. Because of this reason 19 students selected the incorrect choice B where the probability density is zero.

Some undergraduate students (28 out of 95), who used a semi-classical argument in answering the item 17, marked the correct choice. According to this argument the particle has smaller kinetic energy and velocity around the middle of the potential well causing to spend more time in this region. Because of this reason, the amplitude of the wave function is larger than the left and right side of the potential well.

Table 4: Distribution of Undergraduate Level Students’ Answers to the Probability Density of a Particle in a Given Linear Potential Well.

<table>
<thead>
<tr>
<th>Students’ Major</th>
<th>Distribution of the undergraduate students’ responses</th>
<th>Only I</th>
<th>Only II</th>
<th>Only III</th>
<th>I and III</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>N</td>
<td>f   %</td>
<td>N</td>
<td>f  %</td>
</tr>
<tr>
<td>Physics (N=50)</td>
<td></td>
<td>18</td>
<td>36 %</td>
<td>6</td>
<td>12 %</td>
</tr>
<tr>
<td>Physics Education (N=45)</td>
<td></td>
<td>10</td>
<td>22 %</td>
<td>3</td>
<td>7 %</td>
</tr>
<tr>
<td>Total (N=95)</td>
<td></td>
<td>28</td>
<td>30 %</td>
<td>9</td>
<td>9 %</td>
</tr>
</tbody>
</table>

Due to the non-linear potential well, the velocity of the particle is not constant with time. The larger kinetic energy in the right and left sides results in a larger wave number and smaller wavelength for the wave function. Therefore, the wave function behavior must be symmetrically relative to the center of the potential well and the wavelength of the particle decreases when it moves towards the ends of the potential well.

6. CONCLUSION

Our investigation including a multiple-choice test and semi-structured interviews shown that students had various common conceptual difficulties about the potential well phenomenon and probability density of tunneling particles concepts covered in the upper class quantum mechanics courses. Independent of their educational levels (graduate-undergraduate), students share similar difficulties with fundamental concepts such as kinetic energy and total energy of tunneling particles, solution of Schrödinger’s equation in quantum mechanics. In this study, the most common student difficulties were based on the classical mechanics concepts had been identified. These results are
comparable with the study of Morgan (2006) which identified students’ main difficulties in tunneling concept were the ideas which had some traces about classical physics reasoning. Quantum mechanics differs from classical mechanics with its complicated mathematical notation and conceptual scheme. On the other hand, five undergraduate students mentioned that energy was definitely lost during the tunneling process. This result is well known from earlier studies of Morgan et al. (2004) and Redish et al. (2000). Instructional strategies that focus on improving student understanding of quantum tunneling concepts should take these difficulties into account.

REFERENCES


APPENDIX

We reproduce here, as examples, one page from the latest version of the QMCT indicating the standard format of the questions.

10. Assume that the wave function of a free particle is $\psi(\vec{r}, t)$. What is the expression $|\psi(\vec{r}, t)|^2$ equal to?
   
   A) Charge distribution of the particle
   B) Probability amplitude
   C) Position probability distribution
   D) The probability for the particle to be at the position $\vec{r}$ at time $t$.

12. Which one of the following expressions is true for a particle moving in x direction with energy $E(V_0)$ as shown in the figure?

\[ 
\begin{array}{c|c|c|c}
\text{Region I} & \text{Region II} & \text{Region III} \\
\hline
E < V_0 & V_0 & E \\
\end{array} 
\]

A) Total energy in region I is the same as the total energy in region II
B) Kinetic energy of the tunneling particle is the same in region I and in region II
C) Total energy in region I is less than the total energy in region II
D) Potential energy of the particle is decreased.

20. The wave function of a particle is shown in the figure ($|x| \geq 3a$, $\Psi(x) \rightarrow 0$). What is the probability to find the particle between [-2a,-a]?

\[ 
\begin{array}{c|c|c|c|c|c|c}
\text{A)} & 121/161 & \text{B)} & 11/23 & \text{C)} & 121/229 & \text{D)} & 11/26 & \text{E)} & 11/30 \\
\end{array} 
\]
GENİŞLETİLMİŞ ÖZET

Kuantum mekaniği doğanın yasalarına ilişkin fikirlerde paradigma kaymasına sebep olan fizik alanlarından birisidir. Bu nedenle kuantum mekaniği kavramlarının anlaşıl bir biçimde öğrenciлемesi önemlidir (Penrose, 1989) çünkü kuantum mekaniği bilim adamlarına atomik sistemler hakkında hesap ve deneyler yapma imkani sağlayarak bilgi elde etmeyi ve nihayetinde yeni teknolojilerin geliştirilmesine imkan sağlar (Faye, 2002).


Bu çalışma Kuantum Mekaniği Kavram Testi’nin (KMKT) geliştirilmesi ve uygulanması ve uygulanan test sonuçlarına göre seçilen öğrencilere mühalelerin yapılmış olması olarak iki temel kısımdan oluşmaktadır. KMKT seçilen üç üniversitenin fizik ve fizik eğitimi bölümlerinde 95 lisans, 15 lisansüstü öğrenciye uygulandı. Örneğin seçilen 10 öğrenci ile yanı yapılandırılmış mühaleler yapılmıştır. Toplaman nicel verilerin analizinde SPSS (Statistical Package for the Social Sciences) paket programı kullanılmış olup, nitel veriler araştırıcılar tarafından kodlanarak bireysel ve grup uzaşımları olarak analiz edilmiştir.


KMKT testinde bulunan başka bir madde yardımıyla ise, verilen lineer bir potansiyel kuyusunda hareket eden bir parçacığın en uygun dalga fonksiyonunun ne olması gerektiğini sorulmuştur (Şekil 2). Bu sorunun amacı, potansiyel kuyusun içinde hareket etken bir parçacığın kinetik enerjisi ile olasılık...