CLASSICAL-QUANTUM INTERFACE AT UNDERGRADUATE LEVEL: VISUALIZATION OF ‘WAVEFUNCTION’

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Quantum Mechanics (QM) forms the most crucial ingredient of modern-era physical sciences course curriculum at undergraduate level. The abstract ideas involved in appreciating QM concepts are significantly difficult to visualize due to their counter-intuitive nature and lack of experiment-assisted visualization tools. In the heart of quantum mechanical formulation lays the concept of ‘wavefunction’ which forms the basis for understanding behaviour of physical systems. For example, squaring the modulus of ‘wavefunction’ (for a state) provides us the information about probability density which can be used for determining the probability of finding a particle in that state. At tertiary level, the concept of ‘wavefunction’ is introduced in an abstract and mathematical framework which opens up an enormous scope for alternate conception and improper visualization. In the present study, we attempt to explore and comprehend the visualization models constructed by undergraduate students for appreciating the concept of ‘wavefunction’. We present qualitative analysis of a data obtained from administering a questionnaire containing 4 visualization based questions on the topic of ‘wavefunction’ to a group of 10 tertiary-level students of an institute in India which excels in teaching and research of basic sciences. Based on the written responses of students, all the 10 students were interviewed in detail to unravel the exact areas of difficulty in appropriate visualization of ‘wavefunction’.

INTRODUCTION

Quantum mechanics (QM) forms the backbone of present-day physical as well as chemical sciences and its roots have now spread into domains of engineering streams especially in the area of communications. The fundamental concepts and formulations in QM are introduced at undergraduate curricula and in general, these concepts are presented in an abstract and mathematical framework to the students. It is apparent from previous researches in the area of physics education research (PER) that the students face difficulty in understanding various aspects of basic QM which includes probabilistic interpretation of particle’s location (Bao & Redish, 2002), concepts related to probability density (Singh, 2001), measurement in QM as well as time-development of quantum states (Johnston, Crawford & Fletcher, 2007) and many more (Styer, 2008; Singh, 2008; Redish, Bao & Jolly, 1997). An innovative route for assisting students to appreciate quantum mechanical concepts could be achieved by equipping them to ‘visualize’ the problems in QM at the fundamental level (Ayene, Kriek & Damtie, 2011; Greca & Freire, 2014). In addition to its impact on students majoring in physics, visualization of relevant aspects of ‘core-level’ QM problems (such as 1-D finite and infinite potential well, spherically symmetric potential well, Hydrogen-atom problem) would be immensely helpful for students majoring in chemistry (Tsaparlisa & Papaphotis, 2009; Dangur, Avargil, Peskin & Dori, 2014). This could be easily derived by noting the fact that concepts related to orbitals, overlap of orbitals, allowed electronic transitions etc. is a straightforward manifestation of spatial distribution and overlap of eigenfunctions corresponding to identical or different eigenstates (Steinberg, Wittmann, Bao & Redish, 1999).

An important feature of QM lies in the technological difficulty in performing simple experiments which could illustrate underlying QM concepts. Although, there have been attempts made in this direction such as interference using correlated photons, the complexity and sophistication required to perform these experiments renders them impractical for an undergraduate teaching laboratory (Galvez et al., 2005). This results in escalation of difficulty level for students towards establishing a correlation with the classroom teaching with actual or real outcome. This, in turn, could lead to inappropriate visualization of basic QM concepts (Hiller et al., 1995). It has been often found that the visualized models for appreciating QM concepts strongly interfere with the visual frames existing with them for understanding topics in classical mechanics or electromagnetism (Hadzidaki, Kalkanis & Stavrou, 2000). At times, this results in over-simplification of problems and inappropriate understanding. For example, after years of experience in a seemingly deterministic world, reinforced by learning classical physics, students develop a strong deterministic view of the physical world (Paoloni, 2007). On the other hand, the domain of QM considers probabilistic representations to be fundamental to the understanding of physical world which is contrary to the deterministic ones. This may strongly interfere with the process of constructing a consistent mental model amongst students at undergraduate level. This interference of thoughts is an important source for development of alternate framework of concepts in QM (Cataloglu & Robinett, 2002). For example, the concept of ‘wavefunction’ or ‘state vector’ lies at the core of quantum mechanical formulation which is quintessential for obtaining probability, expectation value, uncertainty etc. An improper visualization of wavefunction in terms of its time evolution or physical interpretation could result in incorrect conception of quantum mechanical quantities. Styer, in his seminal work have shown that the students tend to exhibit varied misconceptions in interpreting ‘wavefunction’ or ‘state vector’ from the perspective of its definition and its importance in identifying particle’s motion (Styer, 2001). In the present work, we explore the visualization models constructed by the undergraduate students and the physical interpretation of concept of ‘wavefunction’ or ‘eigenfunction’ of a state. Here, we primarily focus on the students’ visual constructs of the concept of wavefunction and its interpretation in terms of applying them in physics.

OBJECTIVES AND METHODOLOGY

This is a qualitative study in which we have made an attempt to explore learners’ mental models. In order to ascertain the students’ visualization of quantum mechanical ‘wavefunction’, we chose question nos. 5, 6, 9 and 12 from Quantum Mechanics Visualization Instrument or QMVI[1] which is specifically designed for ascertaining students’ visual construct of various QM related concepts (Cataloglu & Robinett, 2002). QMVI is in the form of multiple choice questions with five options out of which only one is correct. In order to identify the conceptual understanding, authors of QMVI have tried to construct questions which primarily involved visual representations of potentials, wavefunctions, energy eigenstates etc. with little or no mathematics. However, the students were needed to appreciate the relationships between various physical variables and their role in determining dynamics (both classically and quantum mechanically) of the system. It is worthwhile to note that content of QMVI substantially matches with QM curriculum adopted by a majority of institutions of higher scientific learning in India and in congruence with the syllabus prescribed by University Grants Commission (UGC), India. Q5, Q6, Q9 and Q12 of QMVI was administered in the form of written test to 10 students (S1 to S10) of National Institute of Science Education and Research (NISER) which is a government-aided institute excelling in teaching and learning of basic sciences. Due permission was obtained from the institution as well as the concerned teacher who was teaching Quantum Mechanics in that semester. Learners were also apprised of the test as well the objective of the study. Their permission was also sought for publishing their data.

At the time of administering QMVI, the students had already credited one course on classical mechanics (includes Lagrangian and Hamiltonian formulation), one basic course in QM (includes solution of Schrodinger equation for various potential functions, wave-packets, time-independent perturbation theory etc.), two courses on electromagnetism (includes static electricity & magnetism, boundary value problems, Maxwell's equations, dipole radiation, special theory of relativity etc.), level-1 course on statistical mechanics (includes basic thermodynamics as well as statistics of classical and quantum systems) and one basic course on condensed-matter physics. Written responses were analyzed question-wise with a focus on thinking and logic adopted by the students. Based on this preliminary analysis, all the 10 students were interviewed in detail so as to identify the existing mental models. The interview was semi- structured in nature which was primarily meant to uncover the method of reasoning adopted by the students which would distinctly elucidate difficult aspects of visualizing 'wave function'. Subsequently, the students' interviews were transcribed. The data of both – written responses as well as interviews was analyzed and presented together as they both formed a logical unit. The analysis was done from a constructivist perspective with an underlying assumption that each individual constructs his/her own knowledge based on their previous experience and knowledge. Therefore, there remains a possibility that the students' constructs could be significantly divergent from well-accepted knowledge of the present era. These divergent constructs are called alternate conceptions or misconceptions and our method of analysis essentially helped in delving into the possible reasons for such misconceptions amongst students' in the area of QM. Hence, the primary objective of this study is to identify and bring out the core issues encountered by the students in visualizing various aspect of the concept related to 'wavefunction'. Our analysis and outcomes indicate towards plausible pedagogic strategies which could be employed for providing a more conducive environment for learning abstract concepts in the subject area of QM.

DATA SUMMARY

The students' written response to Q5, Q6, Q9 and Q12 of QMVI is summarized in Table-1 below. Q5 of QMVI aimed at bringing out student's understanding of 'wavefunction' or 'eigenfunction' for a state or alternately 'state vector'. This question required the knowledge about calculation of 'probability of finding a particle' from the 'wavefunction associated with the state' in equally thick regions in real space. The written responses indicated that an overwhelming majority of students displayed appropriate level of understanding (see Table 1). One student (S7) who chose option (c) identified his mistake during the interview and attributed the choice to temporary lack of concentration. However, probing a solitary concept such as $|\text{wavefunction}|^2$ = probability density, may lead to an incomplete picture about student's comprehension on applicability of the concept of 'wavefunction' in different situations. This point is apparent in the subsequent questions Q6, Q9 and Q12 of QMVI. A noticeable point which emerged out from the interviews was that the students used the term 'probability' and 'probability density' interchangeably. Though, in majority of the cases, the students meant ‘probability density’, they instead used the term ‘probability’. This particular aspect could have been probed better if the interval (d*x*) in the region I, II and III in Q5, would have been unequal.

Q6 of QMVI focused on comprehending the relationship between ‘probability’ and ‘wavefunction’ for a hypothetical representation of wavefunction. Additionally, the question needed understanding of the concept of ‘normalization’ of wavefunction which is quintessential for describing physical reality. The written responses showed that 7 students (S1 and S3-S8) chose the correct option (a) and 3 students (S2, S9 & S10) chose option (d) which could be seen in Table-1. However, in the interview, S9 provided a correct description of the recipe for calculation of ‘probability’ after ‘normalization of wavefunction’ and acknowledged the mistake in his choice. Also, S10 adopted a similar route to obtain the probability but used the ‘|wavefunction|’ while carrying out the normalization, instead of ‘|wavefunction|^{2}’, thereby obtaining a numerical value given in option (a). The existence of an alternate conceptual framework of ‘wavefunction’ was evident in the response (both written and oral) of S2 who said “In order to normalize the wavefunction, the limits for integration or summation would be −2A to +3A (along y) and −2a to +4a (along x)”. This particular response by S2 exemplifies various interpretations made by students when they encounter the terms like ‘area under the curve’. Although the students are introduced to topics such as ‘functions and variables’ at the post-secondary or sophomore level, the understanding of ‘dependent’ variables such as fields and wavefunctions and ‘independent’ variables such as space & time in various contexts still remains a grey area amongst students.

Question no.	[a]	[b]	[c]	[d]	[e]
Q5	0 -	0 -	1 (S7)	0 -	9 ** (S1,S2,S3,S4,S5, S6,S8,S9,S10)
Q6	7 ** (S1,S3,S4,S5, S6,S7,S8)	0 -	0 -	3 (S2,S9, S10)	0 -
Q9	1 (S1)	1 (S5)	2 (S2,S10)	4 ** (S3,S6,S7, S8)	2 (S4,S9)
Q12	0 -	3 (S2,S5, S7)	2 ** (S1,S3)	3 (S4,S8,S9)	2 (S6,S10)
** - Correct response					

Table 1: Summary of students’ responses to Q5, Q6, Q9 and Q12 of QMVI. Figures in brackets indicate the student(s) who chose that option.

One of the major concepts targeted by QMVI includes ‘the correspondence between situations classical and quantum domain’ i.e. a physical interpretation of a quantum mechanical representation. Question numbers Q9 and Q12 were exclusively aimed to investigate this conceptual understanding. In order to obtain the correct answer for Q9, the students needed to appreciate that the 'amplitude of wavefunction' determines the probability of finding a particle and the extent of 'wiggle' or 'frequency of oscillation' of a wavefunction is dictated by its kinetic energy or velocity. In addition, Q9 emphasized on acknowledging the fact that probability of finding a particle is small in those regions where the particle velocity is high. Although, the written response for Q9 indicates that maximum number of students (S3, S6, S7, S8) chose correct option, other options were also given considerable importance by the students (see table-1). While options (a) and (b) were selected by S1 and S5 respectively, options (c) and (e) were chosen by 2 students each (S2, S10 – (c) and S4, S9 – (e)). In the interview, S1 admitted that he could not imagine a situation where 'quantum mechanical' quantities could be used for describing classical situations and therefore, he admitted that he had guessed the answer. When he was provided a few hints, he could relate the definition of probability using '$|\text{wavefunction}|^2$' and made an attempt to correlate the wavefunction to that of some very high excited state of 'harmonic oscillator' problem in QM. He then came out with option (d) as the answer which is the correct one. On the other hand, S5 promptly identified options (a) and (b) to be incorrect, during the interview. She mentioned that option (d) would be the correct one as the probability ($\propto |\text{wavefunction}|^2$) is more in regions where the velocity is least.

However, she could not appreciate the importance of 'change in wiggling' of wavefunction even after many hints and logical assists by the researchers. The response of S2, in the interview, distinctly elucidated an alternate and erroneous understanding that "*the wavefunction depicts the actual motion of the particle"*. Therefore, according to S2, the particle is undergoing an amplified oscillatory motion to the right. Moreover, she adds that the increase in amplitude is a signature of increase in velocity. Both the points mentioned by S2 are incorrect which clearly indicates possible misconceptions that students may hold in QM. S10 acknowledges the fact that the probability of finding the particle is more in regions where amplitude of wavefunction is large but he was unable to connect it to any physically observable movement/motion. He cited the reason as lack of information in the question such as potential, force or energy for appreciating the change in wiggling. Even after substantial assistance in terms of hints such as citing examples of wavefunctions encountered in certain potential distributions, he continued to argue that a comprehensive mathematical formulation was required to relate wavefunction to a physically observable quantity such as velocity or acceleration and that is the only approach to solve the problem.

However, he is unable figure out any route to develop such a mathematical relationship. In case of S4 and S9, the fact that 'wavefunction going to zero at infinite wall' in QM had strong impact which resulted in choice of option (e). Although, the amplitude of wavefunction goes to 'maximum' after the collision with infinite wall created considerable doubt in their mind, they were unable to correlate the wavefunction (in Q9) to any other plausible physical motion of a particle which remains consistent with the sacrosanct condition that 'wavefunction goes to zero at infinite wall'. Also, it is implicit from the respective interviews that the 'wiggle' in the wavefunction does not play any crucial role in determining particle's motion. Amongst the students who chose the correct answer, the reasons cited were similar, with a few resorting to some well-studied examples such as 'harmonic-oscillator' problem. However, during the interview, S6 casted a small doubt regarding his choice as he was unable to appreciate the pictorial representation of the wavefunction on extreme right. The doubt was essentially fostered by the idea that 'how can probability (or wavefunction) go to zero just before or after a maximum value?'

Q12 of QMVI required similar appreciation of 'classical-quantum connection' in a slightly different situation. It is interesting to note that framing of this particular question called for a 'text-to-visualization' approach instead of making a 'visualization-to-text' connection as it was in Q9. Since, the concept targeted was identical to that in Q9, it was quite obvious to anticipate that the pattern of responses would closely resemble each other. However, it was surprised to observe that the responses given by students (for Q12) brought out a substantially contrasting picture. Only two students (S1, S3) chose the correct answer and options (b), (d) and (e) where chosen by 3 students (S2, S5, S7), 3 students (S4, S8, S9) and 2 students (S6, S10) respectively (see table-1).

During interviews, S5 and S7 (who chose option (b)) admitted to have misunderstood the term 'H' which was actually the height from which the particle was dropped. They assumed 'H' to be the distance moved by particle starting from z = 0, according to the figures given in the question. After analyzing the 'amplitude' and 'wiggling' aspects of wavefunction again, both of them concluded that option (c) should be the correct option.

However, S2 reiterated an identical 'alternate' viewpoint as she did in Q9 i.e. *"the wavefunction depicts the actual motion of the particle*". According to S2, the particle, oscillates with smaller amplitude as it begins the motion and the amplitude increases when the velocity is high. Also, she mentioned that the wiggling should not change as the particle travels downwards as acceleration of the particle does not have any relationship with the 'frequency of oscillation' and hence, option (b). All the students (S4, S8, S9) choosing options (d) provided different reasons for their choice. S4 asserted that the problem could be viewed in 'classical mechanics' domain as well as in 'quantum mechanics' domain. Classically, either of the figures III or IV could depict the motion of particle but he could appreciate the significance of wiggling in determining the motion of particle. Upon scaffolding, he figured out the correct answer. However, he thinks, quantum mechanically, figures I and II (Q12) are the correct options as the probability would be maximum at the points where velocity is maximum. He noted this point while making a resemblance to the 'ground-state wavefunction' of a harmonic oscillator. S8 adopted an appropriate route by relating oscillation of wavefunction to kinetic energy of the particle but incorrectly related the argument of 'sine' or 'cosine' function to the frequency of oscillation. For example, he inferred that if 'k' is small in 'sin(kx)' where 'x' is a space coordinate, the frequency of oscillation would be more and vice versa. Due to this, he ended up obtaining an incorrect answer. On the other hand, S9 brought in the concept of 'convexity' from potential energy curves encountered in 'special theory of relativity'. According to him, the 'sharpness of change in the amplitude of wavefunction at the extreme points' gives the measure of 'convexity' and the sharpness of the increase is directly proportional to the convexity.

Although, it was not necessary to bring in the concept of 'convexity' of curve in the present context, it appears that S9 was strongly influenced by previous knowledge in the subject of 'special theory of relativity'. The response of S6 distinctly elucidated a bottleneck in appreciating a concept in QM in the realm of actual experiences made by the students. According to him, since the wavefunction exhibits many zeros (or zero probability) as it wiggles, this does not represent a practical situation of a particle falling from a height 'H'. Classically, the probability of finding the particle is not zero anywhere. When asked about the difference in approach for the Q9 and Q12, he said that he did not consider the zero-crossing of the wavefunction in Q9 as it was not evident from the figure. In the interview, S10 again, expressed his inability to correlate concepts in QM to situations in classical domain and reemphasized that a mathematical framework is needed for this purpose, which he is unsure as of now.

DISCUSSION

Our effort was an attempt to delve into students' conceptualization of the fundamental concept of wavefunction in QM. Students' constructs of wavefunction were investigated through their visualization of these basic concepts and their interpretation both in quantum as well as classical realm using QMVI (Cataloglu, 2000). It was found through the study that students had made varied interpretations of the concept of wavefunction. Amongst the various interpretations, a significant fraction was found out to be alternate as compared to accepted interpretations within the discipline. The most important misconceptions revealed through the study are as follows:

- Wavefunction/eigenfunction depicts actual path of a particle
- Increase in amplitude of an oscillatory wavefunction/eigenfunction implies greater velocity of the particle in that region
- Collision with an infinite wall brings a particle to rest instantaneously
- Acceleration is not related to frequency of oscillation/wiggling for an oscillatory wavefunction/eigenfunction
- An oscillatory wavefunction cannot represent actual motion of particles

Through the interviews of each student, many noteworthy observations came to the fore. It was observed that many students could not correlate pictorial presentation to the physical concept it depicted. For instance, S10 in Q9 and S4 in Q12 could not connect wiggle of wavefunction to any physical concept. A clear implication for pedagogy is to make the connection between the physical concept and its pictorial or iconic depiction clear, strong and unambiguous. The teacher could explicate these connections by presenting to learners, varied perspectives of the same concept (physical, mathematical, pictorial etc.).

A significant revelation from this study was the lack of connection or alternate links between QM and classical mechanics. One noteworthy example is of S1 who in Q9 clearly expressed that he could not imagine a situation where quantum mechanical quantities could express classical system, which shows that he conceptualized QM and classical mechanics to be two independent systems rather than being two ends of a continuum. S2 in the same question perceived quantum mechanical systems from a complete classical lens which led to some crucial misconceptions. She expressed that the pictorial representation of wavefunction is the actual motion of particle and hence, the increase in amplitude should depict increase in velocity. Therefore, according to her viewpoint, figure in Q9 should depict an amplified oscillatory motion to the right. Such issues could be resolved pedagogically by distinctly and unambiguously pointing out the domain of application of concepts which are common to different subjects. In addition, it was observed that a few students used technical phrases such as probability, probability density and wavefunction interchangeably without paying due attention to physical meaning of these concepts. Therefore, it becomes paramount to the teachers to repeatedly lay emphasis on significance and depictions described by terminologies in a science classroom. Possibly, alternate implications due to improper usage of terminologies should be explained in conjunction with suitable demonstration. Also, a few students exhibited confusion in mathematical understanding of dependent and independent variables while carrying out wavefunction normalization.

In conclusion, we present our work where we have made an attempt to add qualitative dimension to the studies related to understanding of the concept of ‘wavefunction’ which is fundamental to the subject of QM. Via this study, we have been able to elucidate that the mental constructs of fundamental concepts are revealed explicitly as well as precisely when the students are required to provide reasons behind their written choices in the form of written as well as verbal explanations. Consequently, this study is aimed at helping physics teachers to design their pedagogy for a more meaningful learning environment for topic of QM, at the fundamental level.

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