PARTICLE IN A CONFINING POTENTIAL: DEVELOPMENT OF CONCEPT INVENTORY AND IDENTIFYING STUDENTS ALTERNATIVE CONCEPTIONS

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The problem of a particle in a confining potential in introductory quantum mechanics is one of the starting points beyond Bohr model to mathematically explore how quantization arises and how with each quantized level a corresponding wave function can be attached via the solution of Schrodinger equation explicitly. This problem offers a wonderful opportunity to identify alternative conceptions of students as they make a transition from the world of deterministic classical mechanics to the world of probabilistic quantum mechanics and start seeing its efficacy in explaining phenomenon at the microscopic level. The effort is to take students from alternative conceptions to physically correct concepts. In this paper, we present the developed concept inventory for a particle confined in a box with rigid walls limited to one dimension. The results of the implementation of the inventory are compared with an expert view for each of the question items validated and tested for implementation. Concept inventory is designed and tested at the undergraduate, Bachelor of Science (B.Sc.) level students, who study these concepts not only within quantum mechanics but also in the solid-state physics course each of credit 4, during their three year, six-semester programme.

INTRODUCTION

Quantum mechanics is a physical theory, which has brought a paradigm shift in the understanding of the matter at the microscopic level, and has made us understand the real world. It is as relevant in the macroscopic world as in the microscopic world, because laws of classical physics follow from the laws of microphysics. It comes up with a good useful theory, which makes physical interpretations plausible and understandable by offering means for quantitative interpretation of experimental observations ((Hadzidaki, Kalkains & Stavrou, 2000; Ashcroft & Mermin 1976; Mott & Jones 1958). It is without doubt a key to understand the fundamental structure of matter, which is a collection of large number of microscopic particles (10^{23}). Even during the study of courses such as solid state physics course learners' come across application of various concepts drawn from quantum mechanics (Kittel, 1985). In 1970, Richard Longini in his book *introductory quantum mechanics for the solid state* (Longini, 1970) underlined the importance of basic ideas of quantum mechanics for atomic binding and for solids. However, the foundation of quantum mechanics is probabilistic in nature requiring epistemological issues, which need to be addressed for converting beliefs steeped in classical mechanics to beliefs of the expert regarding quantum mechanics (Styer, 1996) to appreciate its real life applications which has influenced deeply the technological advances made in the 20th century.

A number of conceptual surveys/inventories in different physics domain, to identify the alternative conceptions have been designed and developed by physics education researchers ((Hestenes, Wells & Schwackhammer, 1992; Thortron & Sokoloff,1998; Maloney, O'Kuma, Hieggelke, & Heuvelen 2001; Krause, Decker, Niska, Alford, & Griffin, 2003; Richardson, Morgan, & Dantzler, 2003; Sharma & Ahluwalia, 2015) to as certain alternative ideas held by the learners which are entirely different from the expert view. Sometimes these alternative ideas form a significant barrier to learning correct expert view. In recent years, many studies have been undertaken on students' understanding and alternative conceptions held in quantum mechanics (Belloni, Christian, & Cox, 2006; Zollman et al., 1999; Zollman, Rebello, & Hogg, 2002; Singh, 2007; Singh, 2001; Muller & Wiesner, 2002; Bao & Redish, 2002, Cataloglu, 2002; McKagan, Perkins, & Wieman, 2010; Wuttiprom, Chitaree, Soankwan, Sharma, & Johnston, 2006, 2008; Sadaghiani, 2005). The exploration and research of such alternative conceptions can help teachers and researchers to know how learners perceive particular knowledge and justify their inferences. The information of alternative conceptions can also be helpful for teachers in deciding their teaching strategies to improve student understanding of the concepts.

In this paper, the development of a concept inventory of quantum mechanics for undergraduate, Bachelor of Science (B.Sc.) three years degree course has been discussed. Further, in the paper students' some alternative conceptions identified on one of the theme of concept inventory is presented.

METHODOLOGY USED

The methodology used for developing the concept inventory on quantum mechanics is explained below. The tool (consisting of only one theme "particle in a box") discussed in this paper is a subpart of the concept inventory (Kaistha, 2014) consisting other themes as well. Table 1 provides the concept profile of this theme which can act as a prerequisite for solid state physics course also.

i. Identification of concept domain

Different quantum mechanics concepts which are required to understand various topics of solid state physics course were identified first.

ii. Identification and defining of themes

After identifying the concepts of quantum mechanics, six themes (i) basics of quantum mechanics (ii) wave particle duality (iii) uncertainty Principle (iv) wave function and Schrödinger equation (v) particle in a box and (vi) Tunneling Effect were selected for the concept inventory.

iii. Delphi Study

To validate the above defined themes a research technique called Delphi Study was used. It involved interactions and discussions with the experts of the concerned field. In this case, the process was carried out with almost ten faculty members of physics department of local undergraduate colleges in Shimla, and one Engineering Institute of Shimla.

iv. Interactive session with students

An interactive session was carried out with the third year students of B.Sc. three years degree course. These students had earlier gone through the quantum mechanics and solid-state physics courses. This session helped us to understand the students' difficulties and ideas in the understanding of quantum mechanics and solid state physics courses and hence designing of the questions.

v. Drafting of multiple choice type questions

The drafting of multiple choice question items of the concept inventory was done by consulting various textbooks and other resources. To get structural validity a draft of concept inventory was sent to 15 experts all teachers in colleges or universities all over the country to check mark and point out any

- deviation from concept specificity of the question item
- ambiguity as regards physical concept involved
- ambiguity of wording and diagrams in the sent items
- choices/ alternative options, which in their opinion are not good distracters etc.

vi. Validity (Item Analysis)

To check the quality of each question item, *item discrimination test*, *item difficulty test* and *point biserial coefficient test* were performed on each question item.

vii. Reliability (Test Analysis)

To check the reliability of the whole test, Cronbach Alpha coefficient test and Ferguson Delta test were performed (Kaistha,2014) The instrument developed on alpha coefficient 0.92, which seemed to be reliable (Nunnally, 1978).

MODE USED

As an exploratory testing, the assessment tool (Appendix A) was administered in the form of pre-test and post-test at the beginning and at the end of the quantum mechanics course to undergraduate students. This course was taught to them in the second year of their three years degree (B.Sc.) program by traditional classroom methodology. 128 undergraduate students (UG), studying in four different undergraduate colleges of Shimla, affiliated to Himachal Pradesh University, Shimla, India, participated in it. The tool was also administered to 25 postgraduate (PG) students, studying in Physics Department, Himachal Pradesh University, Shimla. The PG students study an advance course on Quantum Mechanics in their master's program. Along with it the tool was also administered to 50 teachers, teaching physics in the different colleges all over the country (India), and undergoing a three weeks refresher course in physics, at Academic Staff College (ASC), Punjab University Chandigarh, and Academic Staff College (ASC), Himachal Pradesh University, Shimla. To PG students and to the teachers the test was administered only as pre-test. All the target group members were given two weeks advanced intimation for the administering of the test and they took almost an hour to finish the test.

Theme	**Concept Profile: Topics of Solid State Physics course in which concept(s) is/are of theme used**
Particle in a box	Free electron theory of metals, Somerfield's quantum theory of free electron gas model, lattice vibrations, harmonic oscillator, analogy of phonons with photons, band theory of metals and nano science

Table1: Concept Profile of theme-'particle in a box'

DISCUSSION AND ANALYSIS

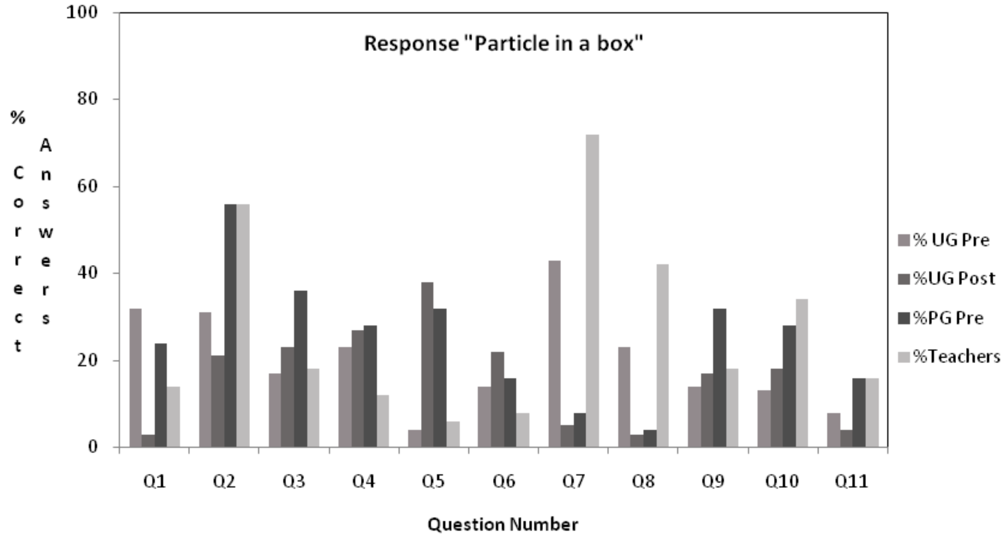

Figure 1: Response of UG, PG students and Teachers on Theme (Particle in a box)

Particle in a box

Particle in a box is a very interesting model in Quantum Mechanics which is mainly used as a hypothetical example to illustrate the differences between classical and quantum confined systems. It is also one of the simple Quantum Mechanics problems, taught in undergraduate physics courses and can be solved analytically without approximations. For example in case of metals, while explaining free electron model, the situation obeyed by particle in a box is used. It is assumed there that conduction electrons are free of the influence of local electric field of atomic origin; however, they are kept inside by the strong forces. Thus, potential is assumed constant inside the material and very large at the surface of metals and holding the electrons inside. Also in explaining Kronig Penny Model which is an idealized one dimensional model of a crystal and exhibits many features of the electronic structure of real crystals, having potential energy of an electron in an infinite sequence of periodically spaced square wells, this concept is used.

The assessment tool on theme **"particle in a box"** involved eleven questions and was administered to UG, PG students and teachers. Figure1 gives the response on the tool by UG, PG students and teachers.

Q1 was based on the fact that, zero energy leads to undefined wave function. 24% of PG students, 14% of teachers and 32% of UG students gave the correct answer in the pre-test. The score of UG students came down to 3% in the post test. Q2 was to compare the ground state energies of hydrogen and helium particles using their masses and to see how energy changes with mass. The percentage of correct answers was 56% for both PG students and teachers, whereas, for UG students percentage was 31% in the pre test which reduced to 21% in the post test. In Q3 students were supposed to differentiate between the dependence of energy on one (n) quantum number, two quantum numbers ($n_{x,}$ n_y) and three quantum numbers ($n_{x,}$ $n_{y,}$ n_z), to check manifestation of degenerate energy levels. Both PG students as well as teachers scored very less in it 36% and 18% respectively. UG students scored 17% in pre test which was increased to 23% in post test. In Q4 students were asked to compare three systems; proton, electron and a billiard ball for lowest energy. In this question, teachers scored 12% less than both UG (23% in pre test and 27% in post test) and PG students (28%). In Q5 students were supposed to appreciate the fact that for a particle in a box, negative value of n in k= nð/L makes "x negative and n=0 makes wave function zero and hence, not possible. Both UG students and teachers scored very less (4% and 6% respectively) than PG students 32%. However, in post test UG students scored 38%. In Q6 solution of Schrodinger equation for a particle in a box in an interval (0, a) was asked. Again, the score of teachers (8%) was less than both UG (14% in pre test and 22% in post test) and PG (16%) students. Q7 to Q11 were graphical questions. In general it was found that students as well as teachers found these graphical questions difficult and scored quite less. Q7 dealt with solving time independent Schrodinger equation for a particle in a square well of width "a". Here teachers scored 72% but scores of both UG (43% in pre test and 5% in post test) and PG (6%) students was very less. in Q8 solution of time independent Schrödinger equation for an infinite square well cantered at the origin was asked. All these questions Q6, Q7 and Q8 required the application of appropriate boundary conditions and then finally normalizing the wave functions.

Q.No	Concept	Alternative Conceptions/misconceptions identified in response to the questions and interviews held later to know how students arrived at their marked responses.
1.	Particle in a box	The energy of bound state and unbound state is same. Students did not have idea that, in bound state problems, energy is found to be quantized & in unbound state, where particle is not trapped, particle will travel as a travelling wave of amplitude Ψ
2.	Ground state energy of H_2& He	Ground state energy of hydrogen and helium is same. No notion that for ground state since the mass of helium is more than hydrogen therefore energy is less
3.	Degeneracy of energy level	Meaning of degeneracy was not clear
4.	Energy level of different systems	Not able to see the Relationship between energy and length of confinement
5.	Allowed boundary conditions	No idea that if n=0 is taken then Ψ and hence probability will become zero & if n is negative then uncertainty principle will give Δx negative, which is not possible.
6.	Wave function from Schrödinger equation	It should vanish at boundaries
7.	Time independent Schrodinger equation for infinite square well	Found difficulties in interpreting meaning of boundary conditions
8.	Time independent Schrodinger equation for infinite square well at origin	Shifting of coordinate system to origin does not have any effect on solution of Schrodinger equation
9.	Relationship between wave number & wave function	Found it difficult to relate wave number & wave function
10.	Probability of finding the particle	Probability amplitude is a place where possibility of finding the particle is most. At center probability is maximum
11.	Expectation value of position	Probability density & expectation value are the same

Table 2: Alternative conceptions in various concepts of Theme "Particle in a box"

After the administration of the tool, to find out why the students have ticked a particular option while attempting the question item of the inventory and also to get an idea of their thinking process interviews were also conducted. We chose 36 UG students of one of the undergraduate colleges and 25 PG students of Physics Department, Himachal Pradesh University for this purpose. Table 2 gives alternative conceptions identified in various concepts of Theme “Particle in a box” in UG and PG students.

CONCLUSIONS

Alternative conceptions originate due to various personal experiences, observations perceptions and prior knowledge which students bring with them in the class room. They are hard to change and may create conflict with knowledge presented by conventional teaching. A student may make sense of the new information in terms of his/her own alternative way of thinking about the topic. Instructional approaches that assess students understanding of the concepts and change their alternative conceptions can act as an effective tool in the classrooms. Physics Education Research based diagnostic assessment tools play an important role to improve student learning as they help to improve their conceptual knowledge. Sometimes, teachers, overestimate our students’ prior knowledge without checking the reality, and try to build new knowledge on a shaky foundation. Introductory undergraduates’ classical physics courses focus on realist perspective and explain both present and future properties of a classical system. However, such a perspective becomes problematic for introductory quantum mechanics learner and hinders the understanding of the same models applied elsewhere for example in solid state physics course. The objective of the present work was to develop and design a validated and reliable assessment tool to investigate students’ understanding of quantum mechanics concepts which may be used prior to the teaching of courses such as solid state physics.

In this paper, statistical analysis, based on the sample of 128 UG students, 25 PG students and 50 teachers was presented which indicated that both students as well as teachers had limited and superficial understanding of fundamental concepts involved in the understanding and usage of ‘particle in box’. This exploratory study brought out alternative conceptions held not only by students but by teachers as well which also reflects on the need for teacher orientation also towards correct concepts In case of UG students we found that traditional lecture based teaching methodology was not effective enough to change their conceptions. This obtained information in this theme could become the basis for developing some teaching aids and further exploration in improving the ground situation. Technology based environment like the one simulations of certain phenomenon can be used as the pedagogical vehicle to increase the content knowledge (Sharma & Ahluwalia, 2012) and to resolve a false notion about the concept.

Future plans

In future we intend to do more intensive study by modifying some of the question items of the concept inventory focusing on addressing the alternative conceptions held by the students and then administer it again to UG and PG students for further analysis.

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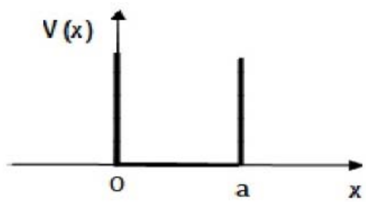
Appendix

1. A particle will not exist inside a rigid box if its energy is:



(a) zero (b) ∞ (c) < 0 (d) > 0

2. Ground state energy of Helium atom in an infinite rigid box as compared to ground state energy of hydrogen atom is:
   (a) higher (b) lower (c) equal

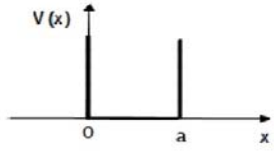
3. A particle will have degenerate energy levels in:
   (a) a one dimensional box (b) a square two dimensional box (c) a cubic three dimensional box

4. The lowest energy level for a electron in a box of length $5.0\text{x}10^{-10}$ m, a proton or a neutron of mass $1.67\text{x}10^{-27}$ kg in a box of width of nucleus ($L= 1.1\text{x}10^{-14}$m) and a billiard ball (m= 0.2 kg) bouncing back and forth between the cushions of frictionless perfectly elastic billiard table (L=1.5m) will be
   (a) $1.69 \text{ x } 10^{6}$eV, 1.5 eV, $7.5\text{x}10^{-48}$ eV (b) $7.5\text{x}10^{-48}$ eV, 1.5 eV, $1.69 \text{ x } 10^{6}$eV,
   (c) 1.5 eV, $1.69 \text{ x } 10^{6}$eV, $7.5\text{x}10^{-48}$ eV

5. For a particle in a box, we choose $k=n\ \pi/L$. To fit the boundary condition that $\psi = 0$ at $x = L$. The values of n are :
   (a) n = 0,-1,-2,-3,…… (b) n = 1,2,3,……. (c) n = 0,1,2,3…….

6. The solution of Schrödinger equation for a particle in a box on the interval
   x = [0,a] is
   (a) $\psi = (\sqrt{2}/a) \sin (n\pi x/a)$ (b) $\psi = (\sqrt{2}/a) \cos (n\pi x/a)$ (c) $\psi = (\sqrt{2}/a) \tan (n\pi x/a)$

7. An electron is confined to a one-dimensional, infinitely deep potential energy well of width a depicted below.
   $V(x) = 0$, *for* $0 < x < a$
   $= +\infty$, *for* $x < 0, x > a$



Solution of the time-independent Schrödinger equation with appropriate boundary conditions for this square well is

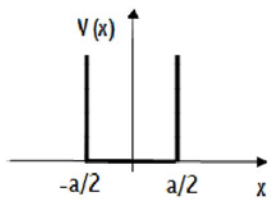
(a) $\varphi_n(x) = (\sqrt{2/a}) \sin (n\pi x/a)$; n=1,2,3…….. (b) $\varphi_n(x) = (\sqrt{2/a}) \cos (n\pi x/a)$; n=1,2,3……..

(c) $\varphi_{n(x)} = (\sqrt{2/a}) \tan (n\pi x/a)$; n=1,2,3…….

8. How does your answer change for the infinite square potential well cantered at the origin?

V (x) = 0, for — a/2 < x < a/2

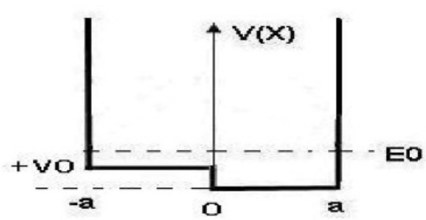
= +∞, for x >a/2



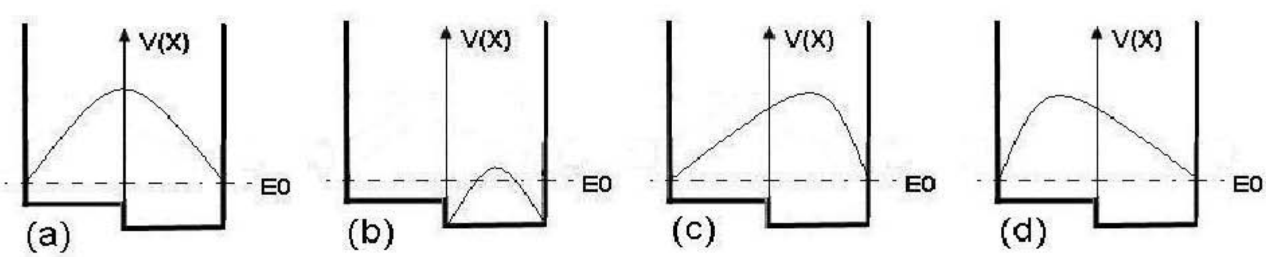
(a) $\varphi_{2n-1} = (\sqrt{2/a}) \sin (n\pi x/a)$; n=1, 2, 3……. b) $\varphi_{2n-1} = (\sqrt{2/a}) \cos (n\pi x/a)$; n=1,2,3……..

(c) $\varphi_{2n-1} = (\sqrt{2/a}) \tan (n\pi x/a)$; n=1, 2, 3……

9. The plot below shows a potential energy function V(x) versus x, corresponding to an asymmetric infinite well. The infinite well is of the width 2a, with impenetrable walls at x= a but where V(x) = + Vo for x between (-a, 0) and V(x) =0 for x between (0, +a)



Of the figures below, which is /are more most likely to be physically acceptable energy eigenstate solutions for the time-independent Schrödinger equation for this well ?

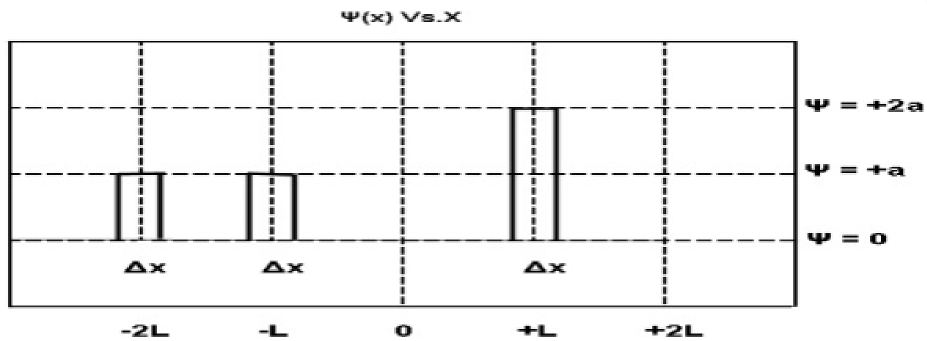


(a) b (b) a (c) d (d) c

10. Consider an infinite square well of width L with a single electron in it. If someone performs a measurement of the electrons' energy and tells you that they found the electron to have energy of n=2 eigenstate, at what positions is the electron most likely to be found?

(a) L/2 (b) L/3, 2L /3 (c) L/4, 3L/4 (d) 0, L/2, L (e) probability is same everywhere.

11. The figure below shows a plot of a wave function $\psi(x)$ versus x, over the range of (-2L, +2L). The wave function vanishes for all other values of x. What is the expectation value of x?



(a) $< x > = 4L/6$ (b) $< x > = - L$ (c) $< x > =0$ (d) $< x > = L/6$ (e) $< x > = - L/4$