International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 7 Issue 9, September - 2023, Pages: 51-56

Teaching quantum particles in one and three-dimensional boxes

Jizreel Pereira da Silva
School of Education, International University Center, Paraná, Brazil
jizreelsilva@yahoo.com.br
Orcid ID: https://orcid.org/0000-0002-7874-1648

Abstract: *The work was developed with the purpose of showing the difficulties of teachers and schools for the insertion of topics of modern and contemporary physics in high school and showing the importance of its use to adapt to the social reality. We present the theoretical development developed in the classroom, with appropriate tools to the accessible language, showing the aspects of energy and probability of the particle in a region configured for the work in question. After the theoretical treatment, operations were developed with virtual experiment so that the students perceive in a visual way, the descriptions of the equations proposed to solve the determined functions. We analyze procedures and discuss the results. Finally, we consolidated the belief in the use of alternative methods in the classroom, showing the motivation of the students for the introduction of the theme, where they had initial contact of quantum mechanics, although we once developed topics of the old quantum mechanics, such as Heisenberg's uncertainty principle, Planck's constant, photoelectric effect, and Bohr's atom.*

Keywords: particle; unidimensional; three-dimensional; energy; box.

1. Introduction

Society is increasingly modernizing with technological innovations, artificial intelligence, among other methodologies that seek to facilitate social life, reducing time for activities that would require more time.

The school receives this consequence of what happens in society and automatically forces the school and teachers to obtain alternatives for their didactic activities so that teaching becomes attractive and effective.

For the case of this work, we began the discussion with the difficulties presented by teachers and schools for the insertion of themes of modern and contemporary physics in high school, presenting the theoretical apparatus in its development, obviously working with mathematical tools suitable for students, ending with the virtual experiment carried out by the students of the 3rd year of a class of a public school in São Cristóvão-RJ, consolidating the discussions with analysis of the results.

2. Difficulties to Insert Quantum Mechanics Topics in the Educational Process

There are many challenges that schools and teachers face in inserting quantum mechanics topics into the educational process. For those who managed to insert themes of this nature, they certainly continue to face problems, such as adequate material, didactic transposition, and equipment for the use of experiment and even the low number of programs that deal with subjects on Modern Physics.

There are several justifications for the use of quantum mechanical topics, such as the recognition of Physics as a human enterprise, awakening and increasing curiosity on the part of the student, presentation of current Physics and its world of research and attraction of young people to the scientific career. [1]

For Terrazzan the physics of high school developed in the classroom is from the period from 1600 to 1850 and for Garden, War and Chrispino:[2][3]

> Focused basically on studies that go little beyond classical mechanics, High School Physics does not present motivating agents for a student who is faced with a physics that is not willing to discuss or modify and does not allow him to understand the actuality that is exposed to him in everyday life. Scientific questions more interesting to this student can be found on the internet, magazines, reports shown in television news and television documentaries (...), but not in the classroom. This distance seems inconsistent with current interests. In addition to the PCN+ and the motivation generated in the students, the teachers also share the ideas of teaching FMC in the classrooms as the importance of a Physics that is extremely necessary to understand the great theoretical and technological innovations of today and that could bring more meaning to learning in the classroom [3].

There is a consensus among researchers who are dedicated to thinking about treatment in the educational context on modern topics of physics. Through interpretive research in relation to the contents of books that address themes of this nature, thought experiments are conceptual tools that enable the study of the physical world by scientists. It is observed the presence of relativity and quantum mechanics in its majority and that have undergone language adaptations, but with content strongly for scientific dissemination.

In the belief of Pospiech cited by Silva and Almeida, he believes it is impossible to talk qualitatively about quantum theory, due to the need to develop concepts and terms through the daily experiences of students, because he believes that language would only be appropriate if it were to use concrete physical objects. Pospiech defends the discussion of philosophical aspects, such as the questions of reality and objectivity of nature.

Paulo and Moreira, cited by Silva and Almeida, sought to analyze how high school students would construct fundamental quantum concepts. After the application of the didactic methodology, the students believed that in science there are no absolute truths.

In the case of teachers, regarding their conceptions about the teaching of Modern Physics in high school, some teachers still do not treat it with priority. Their claims are due to the scarcity of time, the large amount of content to be worked on. They believe they have difficulty transposing the equations and their structure in an accessible way, in view of the perception of the predominant mathematical formalism. In other cases, they believed they did not have autonomy for the didactic treatment [4].

There are teachers who believe that to insert Modern and Contemporary Physics in high school should close all classical physics content. Other teachers believe that students encounter difficulties in their bases, so they do not believe it is possible to treat quantum theories [5].

Based on all this reality, this work aims at an introduction of quantum theory through the treatment of particles in a box with one and three dimensions, through the experimental use of a simulation.

3. PARTICLES IN ONE AND THREE-DIMENSIONAL BOXES

There are several systems that address the regime of quantum mechanics, such as the harmonic oscillator, hydrogen atom, where they can be treated to the problem of a particle.

For this work, it was developed in the application of the model of a particle in the one-dimensional and three-dimensional box. The particle is confined to a certain region of space, in the absence of potential acting on it, but the only action of the potential occurs through the obstacles in the trajectory of the particle.

In the initial discussion, it can be used for the solution of the particle in the box by the principle of minimum action by Wilson and Sommerfeld, obviously for the quantum treatment. The action *S* is given by the product of energy with time or the product of momentum with the position of the particle, where we have in the form

$$S = \int_{t_i}^{t_f} L.dt = \int_{q_i}^{q_f} p.dq \tag{1}$$

Where *L* is the Lagrangian function, *t* the time, *q the* generalized coordinate of position, and *p* the linear momentum.

In the early days of the study of the quantum regime, we used Heinsenberg's uncertainty principle, Planck's constande, Bohr's quantization of angular momentum, and De Broglie's equation. Taking advantage of these early ideas, Wilson and Sommerfeld worked on the sense that allowed steady states should obey the relation of the product of the quantum number n_x to Planck's constant by the integral of momentum and the generalized coordinate. This relationship is nothing more than the trajectory of the particle until its return at the initial point.

So, if we consider a particle confined in a region of space moving in a single direction and in both directions (forward and backward), observing this movement on the x-axis, being the width of the box *a*, we can affirm that outside this region the particle cannot be found.

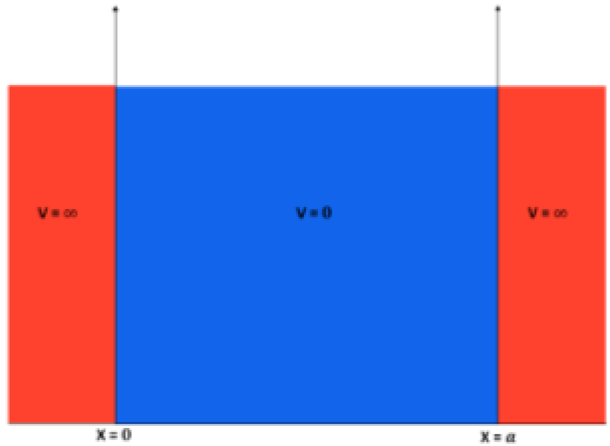


Fig. 1. Infinite potential barrier outside the boundaries of the box [6].

Since the goal is to study the behavior of this particle in this region and the idea would be to prevent the particle from escaping from this range of length, then it is imposed that it feels the effect of an infinite potential. Within the interval $x = 0$ and $x = a$, the potential is zero and the particle can move freely without any force acting on it. In this case the energy of the particle is the kinetic energy, represented by the Lagrangian function of the system, in the form

$$L = E = \frac{mv^2}{2} = \frac{p^2}{2m} \tag{2}$$

Let m be the mass of the particle and v its velocity. When we use the relation of the wavelength given by the De Broglie equation, with, substituting in equation (2), we have $p\lambda = h$

$$E = \frac{h^2}{2m\lambda^2} \tag{3}$$

In the round-trip trajectory of the particle in this box, the preservation of the wave will not be affected, since there is no destructive interference effect, that is, the constructive construction is satisfied if the wave describes a dynamic behavior, presenting an identical value when completing a complete cycle in the system, where the distance $2a$ must be related in the form. Isolating and substituting in equation (3), we present the equation for the energy of the particle confined in a one-dimensional box, in the form $n\lambda = 2a\ \lambda$

$$E = \frac{n^2h^2}{8ma^2} \tag{4}$$

Where we observe that the equation expresses the dependence of the value *of* n, for quantized values of energy. As we increase the dimensionality of the problem, we will follow the same reasoning. And for the case of this work, for three dimensions, we will have in the form

$$E_{x,y,z} = \frac{1}{2m}\left[{p_x}^2 + {p_y}^2 + {p_z}^2\right] + \frac{{n_x}^2h^2}{8ma^2} + \frac{{n_y}^2h^2}{8mb^2} + \frac{{n_z}^2h^2}{8mc^2} \tag{5}$$

Which sets up an isolated particle model [6]. Returning to the case of a particle in a one-dimensional box, making an analysis for the solution, we find that within this configuration, it corresponds to a stationary solution, that is, it does not change with time and is then obtained by the time-independent Schrodinger equation in the form , where the Hamiltonian operator is given by the sum of kinetic and potential energy, in the form $\hat{H}\Psi(x) = E\Psi(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{{d_x}^2} + \mathrm{V}(x)\Psi(x) = E\Psi(x) \tag{6}$$

The particle lies in the potential well, being zero inside and infinite outside the box, where the possibility of analysis is between 0 and a, so the potential is null, and the Schrodinger equation will only have the kinetic energy term in the form

$$\frac{d^2\Psi(x)}{{d_x}^2} = -\frac{2mE}{\hbar^2}\Psi(x) \tag{7}$$

We can use any kind of function to describe this differential equation. For example, we can take and by deriving twice this function and substituting in equation (7), we get. Defining $\Psi(x) = Asin(kx)\frac{2mE}{\hbar^2} = k^2k$ in place of *n, we* substitute in equation (4) and verify that for, we will have in the form$\Psi(x)$

$$\Psi(x) = Asin\left(\frac{\text{n}\pi\text{x}}{a}\right) \tag{8}$$

Let the amplitude *A be* determined by the normalization condition of the function defined as

$$1 = \int_0^a \Psi^*(\text{x})\Psi(x)dx = \text{A}^2\int_0^a \sin^2\left(\frac{\text{n}\pi\text{x}}{a}\right)dx \tag{9}$$

This relation shows the probability of finding the particle in the interval of 0 and *a, by the* maximum value of 1, being given by the normalization condition. By solving the definite integral of equation (8), we determine the value of the amplitude *A* and obtain the normalized wave function, in the form [7]

$$\Psi(x) = \sqrt{\frac{2}{a}}sen\left(\frac{\text{n}\pi\text{x}}{a}\right) \tag{10}$$

4. Simulational Demonstration and Analysis of Results

Physics teachers should use several tools in their didactics, mainly to insert quantum mechanics topics in high school, such as experimental and computational, considering the difficulties of school.

There are several alternatives to teach using low-cost materials, as well as software, where they emphasize the importance of using the computer in the classroom, because the reasons are: the attractiveness on the part of the students and motivation for the use of the computer, encouragement for the use and easy access to notebook equipment or computer in relation to laboratory materials, intensification of learning through visual use, self-didactic development through the computer [8].

Within this perspective, an experimental work was developed with the use of the computer, being carried out with 23 students, identified from (A, B, ..., W) of a class of the 3rd year of high school in São Cristóvão, RJ. The site is given by the Wolfram demo project, drawn up by Cassy Chen, Rasmi Davu and Isabelle Zelaya [9].

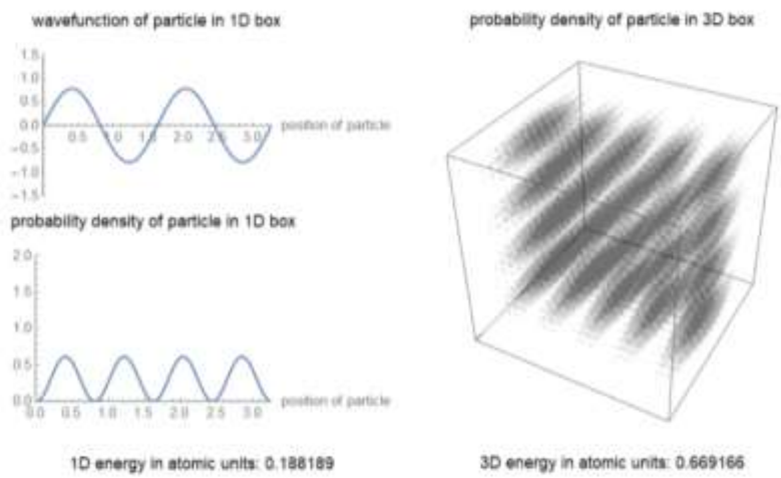
The simulation aims to improve the learning process of students with respect to the description of a particle in the one-dimensional and three-dimensional boxes, where we have the graphs that represent the probability density and energy of the particle. These values will depend on the energy level of the particle and the dimensionality of the box.

The teacher used a notebook, with slide projection on the board in the classroom so that in addition to individually developing their operations, the whole class observes through the projection, the images developed by the student operator of the time.

The students individually performed the operations of manipulation of these variables and observed the influence on the behavior of the particle in the box.

As for the procedure, students in the one-dimensional box part, could put the length of box *a*, ranging from 0 to 10, not limited to integers and quantum number *n* from 1 to 5. For the three-dimensional box, in the same way as the previous item, but for the lengths *a*, b and c, with the quantum numbers n_x, n_y and n_z, also from 1 to 5.

International Journal of Academic and Applied Research (IJAAR)
ISSN: 2643-9603
Vol. 7 Issue 9, September - 2023, Pages: 51-56

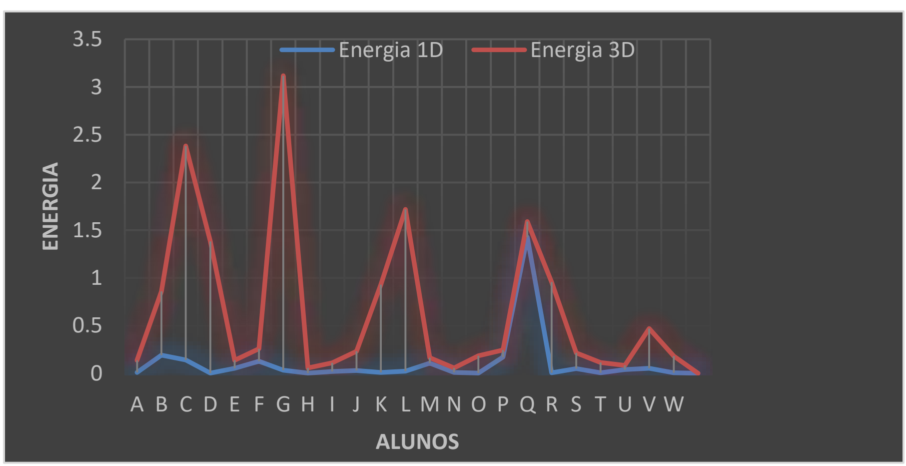


Grap. 1. Student B's operation for the quantum paricle in 1D and 3D boxes.

The graph of the function on the left shows the wave function of the particle in a one-dimensional box and the probability density for a given position. In the graph on the right, it shows the probability density of a particle in a three-dimensional box. In both cases the power value for a given configuration is shown.

In the case of the energy for the one-dimensional box, we noticed that the quantum number (energy level) chosen by the students in the highest choice was 2 and the lowest choice level was 5. For the three-dimensional case, the energy is configured in 3 levels, being in one of the parameters the 5 as the smallest choice and the 3 as the largest choice.

The graph below shows the relationship of the students' configuration to the choice of energy levels for the two cases.



Grap. 2. Operation of student B for the quantum paricle in 1D and 3D boxes.

When we observe graph 1, we notice that student G obtained higher energy in the three-dimensional box and student Q higher one-dimensional energy in their settings. The volume of the cubic region of highest value was with student M.

The students in general, understood the importance of being treated subjects of modern and contemporary physics in the classroom, because there are many open questions in science and even survey of questions on the part of the students about the universe and its daily life, where it is observed the posture of a researcher as a problem solver.

5. Final Considerations

The work sought to highlight the need to insert quantum mechanical topics, in view of the need to adapt to reality. There are difficulties in various segments of the school, because it is still necessary a more solid discussion on the part of the coordinators and teachers for its use, because there are teachers who did not have in their training, contact with modern and contemporary physics and those who had, present a discourse of superficial contact, developing a thought that has no preparation to address themes of this nature in the classroom, nor to think of alternative tools for the didactic process.

In the case of this work, we sought to bring the students closer to the initial contact of quantum mechanics, following the development of the old quantum mechanics through the concepts of the Bohr atom, Heisenberg's uncertainty principle, photoelectric effect, as well as Planck's constant, developed in the works of black body radiation.

The students showed satisfaction and motivation to carry out this work, even considering difficulties for the mathematical treatment, because it is natural the perception of most students a certain difficulty in the mathematical basis in works of this nature.

It is important that teachers and the school believe in this possibility of using alternative tools to improve the teaching-learning process, where it favors students in the absorption of knowledge, as well as for the teacher in his proposal for elaboration in the teaching plan.

6. References

[1] Osterman, F. C., & Moreira, M. A. (2000). A bibliographic review on the research area "Modern and contemporary physics in high school". Investigations in Science Teaching, vol. 5(1).

[2] Terrazzan, E. A. (1992). The isertion of modern and contemporary physics in the teaching of physics in the 2nd grade school. Caderno Catarinense de Ensino de Física, vol 9(3), pp. 209-214.

[3] Jardim, W. T., Guerra, A., & Chrispino, A. (2011). Bibliography review: modern physics and its relevance in high school. In: National Symposium on the Teaching of Physics, vol 18, MA, Brazil.

[4] Silva, A. C., & Almeida, M. J. P. M. (2011). Quantum physics in high school: what the research says. Brazilian Notebook of Physics Teaching, vol. 28(3), pp. 624-652.

[5] Monteiro, M. A., Nardi, R., & Filho, J. B. B. (2009). Difficulties of teachers in introducing modern physics in high school: the need to overcome technical rationality in formative processes. São Paulo: UNESP, Academic Culture, pp. 145-159.

[6] Pereira, G. C., & Custodio, R. (2021). The particle in the box: semiclassical, quantum and numerical solutions. Chemkeys Magazine, vol. 3, e021004, pp. 1-10. DOI: https://doi.org/10.20396/chemkeys.v3i00.15963.

[7] Custodio, R. (2021). Quantum Mechanics. Chemkeys Magazine, vol. 3, e021001. DOI: https://doi.org/10.20396/chemkeys.v3i00.15466.

[8] Sousa, A. C. M., Franco, C. C. C., & Guimarães, K. F. (2013). Learning quantum mechanics in high school through educational software. Journal of Education Research Meeting, Vol 1(1), pp. 5-18.

[9] Chen, C., Davu, R., & Zelaya, I. (2018). Particles in 1D and 3D boxes. Wolfram Demonstrations Project. https://demonstrations.wolfram.com/ParticlesIn1DAnd3DBoxes/.