Complete solutions of particle in three dimensional box with variations in main quantum number

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Abstract. Particle in a box is one of the applications of the Schrodinger equation. Schrodinger equation gives wave function which is used to determine the probability and expectation value of particle in a box. It is also can explain the energy levels of the particle. This study aimed to determine the probability, expectation values, and energy levels of a particle in a three-dimensional box with variations in main quantum numbers in each coordinate axis. The magnitude of the wave function and energy levels are influenced by the main quantum number and the width of the box. The results show that variations in the main quantum number influence the probability of particle in the three-dimensional box except for the width of the box \( \frac{L}{2} \) and \( L \) the probability of particle showing the same value in all variations of the main quantum number. Variations in the main quantum number also influence the expectation value of particle in a three-dimensional box except for the width of the box \( L \) the expectation value shows the same value in all variations of the main quantum number. All variations of the main quantum number also influence the magnitude of the energy level of the particle.

1. Introduction

The universe has things that are macroscopic and some are microscopic. These problems can be solved by physics. One area study in physics is quantum physics. Quantum physics can be used to review microscopic problems as well as particle [1]. The basis or pillar of modern physics is quantum physics. The various problems that exist in quantum physics can be solved using the Schrodinger equation. The Schrodinger equation describes the wave function of a particle [2]. The wave function that results from the Schrodinger equation can describe the dynamic behavior of a particle. The Schrodinger equation can be considered a fundamental equation in quantum field theory [3]. The Schrodinger equation divided into time-dependent Schrodinger equation and time-independent Schrodinger equation. The commonly used equation is the time-independent Schrodinger equation because the equation depends only on position [4].

Some cases in quantum physics can be solved using the Schrodinger equation. One of them is the case of particle in a box. Particle in a box is the simplest case to review. In general, particle in a box is the basic discussion of non-relativistic quantum mechanics. Particle in a box describes the wave nature of particle while showing that the energy of the particle is quantized. The discussion of particle in a box can also be used to review the implications of special relativity for quantum physics [5]. The case of particle in a box can be associated with black body radiation phenomena. Black body is likened to a cavity with a small hole and its relation to the particle in a box, which is this box considered as a
Particle in a box have finite or infinite potential. In general, the particle model in a box for infinite potential boxes is used more often than the finite potential box [8]. Particle in a box certainly have wave functions. The wave function allows the probability of particle in a box to be reviewed. The existence of a probability also allows the determination of the expectation value of the particle. The expectation value is known as the statistical property of a particle [9]. The expectation value can be determined by integrating the probability multiplied by observable X [10]. Particle in a three-dimensional box has an energy level or energy spectrum that is discrete. This is influenced by the main quantum number [11].

This research is a development of previous research. Previous research determined the probability of particle in a three-dimensional box using perturbation theory. In addition, previous research has also been carried out to determine the probability, expectation value, and energy levels of particle in a three-dimensional box with the same main quantum numbers in each coordinate axis [12]. The results of this study will show the probability, expectation value, and energy levels of particle in a three-dimensional box when the main quantum numbers in each coordinate axis are made varied. The limitation of this study is the length, width, and height of the box with the same value of \(\frac{L}{2}, \frac{L}{2}, \frac{L}{4}, \frac{L}{4}\) and \(L\). The length, width, and height of the box use the Bohr atomic radius approach of \(0.5 \times 10^{-10}\) m. This study reviews the particle to the second excited condition \((n \leq 3)\).

## 2. Method

This research is included in the type of theoretical study research which consists of several stages. The steps of the method to get the final results of this research can be written as follows:

2.1 The first steps of the method is to write down the law of conservation of energy

The law of conservation of the energy has the following form of equation:

\[ K + V = E \quad (1) \]

2.2 The second steps of the method is to write down the time-independent Schrodinger equation in three-dimensional region

The time-independent Schrodinger equation can be obtained by reviewing the law of conservation of energy, de Broglie hypothesis, and applying the velocity formula \(v = \frac{\hbar \omega}{p}\). The form of the time-independent Schrodinger equation can be written as follow:

\[ \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{2m}{\hbar^2} (E - V) \psi(x) = 0 \quad (2) \]

2.3 The third steps of the method is to determine the solutions of time-independent Schrodinger equation in three-dimensional region

The time-independent Schrodinger equation in a three-dimensional region will provide a solution. This solution can be obtained by using variable separation techniques. The solution of the time-independent Schrodinger equation in three-dimensional region has the following form of equation:

\[ \psi_{x,y,z} = K(x) L(y) M(z) \quad (3) \]

2.4 The fourth steps of the method is to determine the boundaries of the three-dimensional box

Particle in three-dimensional box has the following restrictions:
\[ V(x, y, z) = \begin{cases} 0, & 0 \leq x, y, z \leq L, \\ \infty, & \text{the others} \end{cases} \]

The area that has \( V = \infty \) is the area outside the box. If the Schrödinger equation is applied to regions outside the box it will give results \( \psi = 0 \). The area that has \( V = 0 \) is the area in the box and it will give the particle wave function.

2.5 The fifth steps of the method is to apply the normalization condition to get the particle wave function

Normalization requirements are:

\[ \iiint_{0}^{L} |\psi|^2 \, dx \, dy \, dz = 1 \quad (4) \]

The application of the normalization conditions will provide the complete form of the particle wave function in a three-dimensional box as follows:

\[ \psi_{x,y,z} = \frac{8}{L^3} \sin \left( \frac{n_x \pi}{L} x \right) \sin \left( \frac{n_y \pi}{L} y \right) \sin \left( \frac{n_z \pi}{L} z \right) \quad (5) \]

2.6 The sixth steps of the method is to determine the probability of the particle in three-dimensional box

The equation for determining the probability of particle in a three-dimensional box is:

\[ \iiint P(x, y, z) \, dx \, dy \, dz = \iiint |\psi|^2 \, dx \, dy \, dz \quad (6) \]

Substitution equation (5) in equation (6) to obtain the following result:

\[ \iiint P(x, y, z) \, dx \, dy \, dz = \iiint \left( \frac{8}{L^3} \sin \left( \frac{n_x \pi}{L} x \right) \sin \left( \frac{n_y \pi}{L} y \right) \sin \left( \frac{n_z \pi}{L} z \right) \right)^2 \, dx \, dy \, dz \quad (7) \]

2.7 The seventh steps of the method is to determine the expectation value of the particle in a three-dimensional box

If the probability that has been obtained is multiplied by observables in the form of positions \((x, y, z)\) then the expectation value of particle in a box can be determined as follows:

\[ \langle V \rangle = \iiint |\psi|^2 xyz \, dx \, dy \, dz \quad (8) \]

By substituting equation (5) in equation (8), the expectation value of a particle in a three-dimensional box is obtained as follows:

\[ \langle V \rangle = \iiint \left( \frac{8}{L^3} \sin \left( \frac{n_x \pi}{L} x \right) \sin \left( \frac{n_y \pi}{L} y \right) \sin \left( \frac{n_z \pi}{L} z \right) \right)^2 xyz \, dx \, dy \, dz \quad (9) \]

2.8 The final steps of the method is to determine the energy levels of the particle in a three-dimensional box

The form of the particle energy levels equation in three-dimensional box can be written as follows:

\[ E = \left( n_x^2 + n_y^2 + n_z^2 \right) \frac{\pi^2 \hbar^2}{2mL^2} \quad (10) \]

3. Result and Discussion

Particle probability is the possibility to find a particle in a box with a certain width. Calculation of probability values can be used to determine the distribution of particle in a box. Particle probability is influenced by several things, including the main quantum number and the width of the box. This research used a three-dimensional box so that the main quantum numbers used were \((n_x, n_y, \text{dan } n_z)\). The variations of main quantum numbers used will also affect the magnitude of the probability. The situation used in this research is the state of the particle to the second excited. The width of the box used is \( \frac{L}{2}, \frac{L}{4}, \frac{3L}{4}, \text{and } L \). Data of particle probability in the three-dimensional box with variations in main quantum numbers are shown in the following Table 1:
| State   | Box Width         | Probability                  |
|---------|-------------------|------------------------------|
| (1 1 2) | $\frac{L}{4}$     | 0,0020595409550              |
|         | $\frac{L}{2}$     | 0,125                        |
|         | $\frac{3L}{4}$    | 0,620032126049738326098421842671 |
|         | $L$               | 1                            |
| (1 1 3) | $\frac{L}{4}$     | 0,0024913449238              |
|         | $\frac{L}{2}$     | 0,125                        |
|         | $\frac{3L}{4}$    | 0,456926614112780379199114807567 |
|         | $L$               | 1                            |
| (2 2 1) | $\frac{L}{4}$     | 0,0056727707006              |
|         | $\frac{L}{2}$     | 0,125                        |
|         | $\frac{3L}{4}$    | 0,3323049363057              |
|         | $L$               | 1                            |
| (2 2 3) | $\frac{L}{4}$     | 0,0189424097664              |
|         | $\frac{L}{2}$     | 0,125                        |
|         | $\frac{3L}{4}$    | 0,3920183121019              |
|         | $L$               | 1                            |
| (3 3 1) | $\frac{L}{4}$     | 0,0083373038888              |
|         | $\frac{L}{2}$     | 0,125                        |
|         | $\frac{3L}{4}$    | 0,39005485222598              |
|         | $L$               | 1                            |
| (3 3 2) | $\frac{L}{4}$     | 0,0229641528166              |
|         | $\frac{L}{2}$     | 0,125                        |
|         | $\frac{3L}{4}$    | 0,3642746240                 |
|         | $L$               | 1                            |

The results of the study show that the situation of $n_x = n_y \neq n_z$, $n_x = n_z \neq n_y$ and $n_x \neq n_y = n_z$, such as (1,1,2), (1,2,1), and (2,1,1) give the same value of particle probability for all widths of the box. Probability shows the same value in all variations of main quantum numbers when the width of the
box used is $\frac{L}{2}$ and $L$. On the other hand, the probability of particle will show varying value for all variations of main quantum numbers when the width of the box used is $\frac{L}{4}$ and $3\frac{L}{4}$. So, variations in main quantum numbers only affect the width of the box $\frac{L}{4}$ and $3\frac{L}{4}$.

The data obtained shows the probability of finding a particle in a box. The data is in the form of numbers. These numbers, when multiplied by 100% will show the percentage to find the particle in a box. For example, when the main quantum numbers variation used is (1,1,2). In this variation, the resulting probability varies for each box width. When the width of the box used $\frac{L}{4}$ the particle probability is 0.206%, for the width of the box $\frac{L}{2}$ the particle probability is 12.5% when the width of the box $3\frac{L}{4}$ the particle probability is 62% and for the width of the box $L$ the particle probability is 100%. It means, if the smaller percentage produced, it will be very difficult to find the particle in a box. On the other hand, if the greater percentage produced, it will be easier to find the particle in a box. In the variation (1,1,2) the particle will be very difficult to find in areas with a width of $\frac{L}{4}$ and will be easy to find in areas of the box with a width of $L$.

When the width of the box used is $\frac{L}{4}$ the smallest probability value shown in the variation of main quantum numbers (1,1,2) which is equal to 0.206%. When the width of the box used is $\frac{L}{4}$ the probability value, in general, continues to increase. When the variation of the main quantum number (1,1,2) the probability is 0.206%, but when the variation of the main quantum number (2,2,1) the probability value increases to 0.57%. When the variation of the main quantum number (1,1,3) the probability is 0.249%, but when the variation of the main quantum number (3,3,1) the probability value increases to 0.83%. When the variation of the main quantum number (2,2,3) the probability is 1.89%, but when the variation of the main quantum number (3,3,2) the probability value increases to 2.296%. Based on this data, the variation of main quantum numbers causes an increase value of particle probability for the width of the box $\frac{L}{4}$.

When the width of the box used is $\frac{3L}{4}$ the smallest probability value shown in the variation of main quantum numbers (2,2,1) which is equal to 33.2%. When the width of the box used is $\frac{3L}{4}$ the probability value, in general continues to decrease. When the variation of the main quantum number (1,1,2) the probability is 62%, but when the variation of the main quantum number (2,2,1) the probability value decreases to 33.2%. When the variation of the main quantum number (1,1,3) the probability is 45.69%, but when the variation of the main quantum number (3,3,1) the probability value decreases to 39%. When the variation of the main quantum number (2,2,3) the probability is 39.2%, but when the variation of the main quantum number (3,3,2) the probability value decreases to 36.4%. Based on this data, the variation of main quantum numbers causes a decrease value of particle probability for the width of the box $\frac{3L}{4}$.

Based on the data obtained, overall it can be seen that the smallest probability is in the variation (1,1,2) with the width of the box used $\frac{L}{4}$ which is equal to 0.206% and the biggest probability is in all variations of main quantum number with the width of the box used is $L$ and percentage by 100%. The magnitude of particle probability in the three-dimensional box with variations in the main quantum number is not only shown by calculation but also supported by visualization with Figure 1 as follows:
Figure 1. Probability of particle in three dimensional box with variations in main quantum number in the width of the box $L^4$, $L^2$, $3L^4$, and $L$ for variations in main quantum numbers (1,2,1).

Figure 1 above shows a graph of the particle probability in the three-dimensional box with variations in the main quantum number of (1,2,1). Each graph shows a different shape. This shows that the distribution of a particle in a box varies between one state and another. Each graph has its own number of peak points. When the variation of main quantum number (1,2,1), the particle has a peak point of 32 for the width of the box used is $L^4$, particle has a peak point of 8 for the width of the box $L^2$, particle has a peak point of 3 for the width of the box $3L^4$, and the particle has a peak point of 2 for the width of the box $L$.

The expectation value of a particle is the expectation of the appearance of a particle in a box. Expectation value is not an actual state, but the average appearance of a particle in the box. The greater expectation value shows that the greater expectation of the appearance of a particle in an area of the box. As same as probability, the expectation value is also influenced by the main quantum number and the width of the box. Variations in the main quantum number will also influence the magnitude of the expectation value of the particle. Data of expectation value of particle in the three-dimensional box with variations in main quantum numbers are shown in the following Table 2:

### Table 2. Results of Calculation of Particle Expectation Values in Three Dimensional Box with Variations in Main Quantum Numbers.

| State   | Box Width | Expectation Values ($L^3$) |
|---------|-----------|---------------------------|
| (1 1 2) | $L^4$     | 0.0000123821610            |
|         | $L^2$     | 0.0042558625883            |
|         | $3L^4$    | 0.0533251497998            |
|         | $L$       | 0.125                      |
| (1 1 3) | $L^4$     | 0.0000133442646            |
|         | $L^2$     | 0.0047709916283            |
|         | $3L^4$    | 0.0443190512682            |
|         | $L$       | 0.125                      |
As same as probability, when the situation of \[ n_x = n_y \neq n_z, \] \[ n_x = n_y \neq n_z \] and \[ n_x = n_y = n_z, \] for example in the state of variation (1,1,3), (1,3,1), and (3,1,1) the expectation value will show the same value for all widths of the box. Variations in the main quantum number affect the expectation value of particle for all widths of the box. The variations of the main quantum number does not affect the magnitude of the expectation value of particle only for the width of the box \( L \), the resulting expectation value is equal to 0.125. When the width of the box used is \( L/4 \) the smallest expectation value is indicated by variations in the main quantum number (1,1,2). When the width of the box used is \( L/4 \) the expectation value of particle, in general, continues to increase. For example, when the variations of the main quantum number (1,1,2) the expectation value of particle is 0.0000123821610, but when the variations of the main quantum number (2,2,1) the expectation value increases to 0.0000323831990. When the width of the box used is \( L/4 \) the expectation value of particle, in general, continues to decrease. For example, when the variations of the main quantum number (1,1,3) the expectation value of particle is 0.0047709916283, but when the variations of the main quantum number (3,3,1) the expectation value decreases to 0.0029965557003. When the width of the box used is \( L/4 \) the expectation value of particle, in general, continues to decrease. For example, when the variations of the main quantum number (2,2,3) the expectation value of particle is 0.0211020321053, but when the variations of the main quantum number (3,3,2) the expectation value decreases to 0.0175516168762.

In addition to influence the magnitude of the probability and the expectation value of the particle in a three-dimensional box, variations of the main quantum number also influence the magnitude of

| State  | Box Width | Expectation Values (L^3) |
|--------|-----------|-------------------------|
| (2 2 1) | \( L/4 \) | 0.0000323831990 |
|        | \( L/2 \) | 0.0027446967470 |
|        | \( 3L/4 \) | 0.0367958632698 |
|        | \( L \) | 0.125 |
| (2 2 3) | \( L/4 \) | 0.0000912727736 |
|        | \( L/2 \) | 0.0020410774162 |
|        | \( 3L/4 \) | 0.0211020321053 |
|        | \( L \) | 0.125 |
| (3 3 1) | \( L/4 \) | 0.0000376111095 |
|        | \( L/2 \) | 0.0029965557003 |
|        | \( 3L/4 \) | 0.0254300120703 |
|        | \( L \) | 0.125 |
| (3 3 2) | \( L/4 \) | 0.0000983647394 |
|        | \( L/2 \) | 0.0021328425866 |
|        | \( 3L/4 \) | 0.0175516168762 |
|        | \( L \) | 0.125 |
energy levels of particle. Data of energy levels of particle in a three-dimensional box with variations in main quantum numbers are shown in the following Table 3:

| Main Quantum Numbers of Particle $(n_x, n_y, n_z)$ | Energy Levels (E) $(x10^{-16}$ J) |
|--------------------------------------------------|----------------------------------|
| 1 1 1                                            | 0.7167170769                     |
| 1 1 2                                            |                                 |
| 1 2 1                                            | 1.4333942246                     |
| 2 1 1                                            |                                 |
| 1 1 3                                            | 2.6278894118                     |
| 3 1 1                                            |                                 |
| 2 2 1                                            | 2.1500913369                     |
| 2 1 2                                            |                                 |
| 1 2 2                                            | 4.0612836364                     |
| 2 2 3                                            |                                 |
| 2 3 2                                            | 4.5390817112                     |
| 3 2 2                                            |                                 |
| 3 3 1                                            |                                 |
| 3 1 3                                            |                                 |

Table 3. Results of Calculation of Particle Energy Levels in Three Dimensional Box with Variations in Main Quantum Numbers.

The energy levels of particle show the same value at certain variations of the main quantum number. The energy levels of the particle shows the same value for the situation of $n_x = n_y \neq n_z$, $n_x = n_z \neq n_y = n_z$, and $n_x \neq n_y = n_z$. In this situation, in general, particle degenerate three times. Particle also have more energy than their basic state. This is because particle excite or move to other atomic shells. The results of this research also shows that the energy levels of the particle will be greater if the main quantum number that is varied or combined is also higher. This is because the particle needs more energy if it is farther away from the nucleus.

4. Conclusion

Things that can be seen from the case of particle in a box are the probability, the expectation value, and the energy levels. This research used three-dimensional box. The results showed that the probability, the expectation value, and the energy levels of particle were influenced by the main quantum number and the width of the box. In addition, variations of the main quantum number also influence the magnitude of the probability, the expectation value, and the energy levels of particle. The results show that for all variations of the main quantum number, the probability of particle shows varying values on the width of the box $L$ and $\frac{3L}{4}$. For all variations of the main quantum number, the expectation value of the particle shows varying values except for the width of the box $L$. The energy levels of the particle generally shows the same value for the situation of $n_x = n_y \neq n_z$, $n_x = n_z \neq n_y = n_z$, and $n_x \neq n_y = n_z$. These variations show that the energy levels of particle in a three-dimensional box with variations in main quantum numbers are shown in the following Table 3:
\( n_y \neq n_x = n_z \). The energy levels of the particle will be greater if the main quantum number that is varied or combined is also higher.

The strength of this research can review particle in a partially excited state. However, this research also has the weaknesses of not being able to provide complete or thorough results because the area being reviewed is only in one form and the condition is used only until second excited. The magnitude of the probability, the expectation value, and the energy levels of the particle in differently shaped regions will give different results. This research has used a cube-shaped box. So, further research can review particle in regions that are not cuboidal, which are regions that have different lengths, widths, and heights of the box. Besides that, different particle states will give different results. This research has used conditions ranging from ground conditions to the second excited state. To obtain maximum and thorough results, further research can use more conditions than the second excited state \((n > 3)\).

**Acknowledgment**

We gratefully acknowledge the support of 3rd Research Group Physics Education from FKIP-University of Jember of the year 2019.

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