Determination of energy levels, probabilities, and expectation values of particles in the three-dimensional box at quantum numbers $\leq 5$

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Abstract. Static potential boxes represent an area that is limited by an infinite potential wall, where there is no external potential in it. The solution of the Schrodinger equation gives a wave function that can explain the energy level and determine the probability of finding a particle at any point. The main focus of the research in this paper was to solve the solution to the energy levels, probabilities, and expectation values of a particle in a three-dimensional box, where control limits are given for the potential box width, namely $L/4$, $L/2$, $3L/4$, and $L$ for each situation. In this research, the results showed that probability meetings depend on changes in box width and quantum number of particles, while particle energy levels depend on the length of the box and the quantum number of particles. Based on the relation between probabilities and expectation values, the most stable size of the box to find the particles in ground state to the fourth excitation state is at the width of $L/4$ and $L$.

1. Introduction

Potential wells or potential boxes are one form of particle system modelling that moves in space with simple potential and bound quantities. The potential box is classified into 2 parts, namely the static potential box and the dynamic potential box. The static potential box represents an area which is limited by an infinite potential wall, where there is no external potential in it. Whereas a potential dynamic box represents an area that is almost the same as a static potential box, but the difference is that one of the walls moves at a constant speed $v$.

Schrodinger's general equation is one simple form of equation used to solve quantum physics problems which explain in detail the interactions between electrons and atomic nuclei [1]. Based on the general characteristics of the wave function, the Schrodinger equation is classified into 2, which is dependent on time and independent of time (free of time or steady state) [2]. The independent time Schrodinger's equation is one of the equations used to solve cases that are closely related to the study of potential boxes, both potential static and dynamic boxes. The solution to the Schrodinger equation produces a wave function $\psi(\vec{r}, t)$ which is a function of two variables, space and time. This wave function can be used to explain the particle's energy level and $|\psi(\vec{r}, t)|^2$ can be interpreted to determine the probability of finding particles in any point.

The wave function and energy of a particle mass $m$ in a potential box are usually represented in a one-dimensional state. Research on wave function and particle probability in one-dimensional potential boxes with the Klein-Gordon equation produces the same final wave function as the use of the Schrodinger equation [3]. The energy level value in a semiconductor quantum well can be obtained through the analysis of a potential one-dimensional box [4]. When variations in the width of the well are reduced by the potential energy remaining in the one-dimensional potential box, the energy level and wave function are obtained with 2 conditions. If given the width of the well is large, then no energy level or wave function can be seen [5]. In the case of a one-dimensional potential box, the result is that the particle state will always end in half a box that has a wider size after the splitting process is
done [6]. The transition probability shows oscillating behaviour, the more complex the particle state will affect the amount of oscillation behaviour [7].

This research develops previous research on particles in a one-dimensional box, where the solution to this case will give the results of the wave function and the value of the energy level of a particle[8]. Another advantage of this research is the determination of the probability value of a particle in a potential three-dimensional box on the ground state, first excitation, second excitation, third excitation, and fourth excitation. In addition, the renewal of this study is the calculation of expectations and control of the potential box width, namely \( \frac{L}{4} \), \( \frac{L}{2} \), \( \frac{3L}{4} \), and \( L \) for each state, where previously only reached \( \frac{L}{4} \) The side length of the box (\( L \)) in this research is based on the approach of the radius hydrogen atom in Bohr atomic theory, which is 0.5 Å or \( 0.5 \times 10^{-10} \) m. The limitations given in this research are the values of quantum numbers \( n_x, n_y, \) and \( n_z \) in each situation made the same.

2. Method

Obtaining the wave function equation and particle energy in a three-dimensional potential box is based on equation (1) which is the total particle energy equation \( E \) (summation of kinetic energy \( K \) with potential energy \( V \)) [9]:

\[
E = K + V
\]  

(1)

Each potential three-dimensional box wall has a very high potential value (\( V \to \infty \)), but the potential in the box is zero (\( V = 0 \)). The amount of particle kinetic energy value \( K = \frac{(p_x^2 + p_y^2 + p_z^2)}{2m} \), where the value \( (p_x^2 + p_y^2 + p_z^2) \) is \((-\hbar \nabla)^2\) with \( \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \) so that the total energy value \( E \) of particles is obtained in the potential three-dimensional box as follows

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

(2)

By substituting the function \( \psi \) into equation (2), the Schrödinger equation of the particle in the potential three-dimensional box is obtained as follows

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

(3)

Then the method of separating the wave function variable and energy is done in equation (3)

\[
\psi(x,y,z) = X(x)Y(y)Z(z)
\]  

(4)

and

\[
E = E_x + E_y + E_z
\]  

(5)

So that is obtained

\[
\frac{\partial^2 X(x)}{\partial x^2} + \frac{2m}{\hbar^2} EX(x) = 0
\]  

(6)

with

\[
X(x) = A \sin k_x x + B \cos k_x x
\]  

(7)

\[
\frac{\partial^2 Y(y)}{\partial y^2} + \frac{2m}{\hbar^2} EY(y) = 0
\]  

(8)

with

\[
Y(y) = C \sin k_y y + D \cos k_y y
\]  

(9)
\[ \frac{\partial^2 Z(x)}{\partial z^2} + \frac{2m}{\hbar^2} E Z(x) = 0 \]  

(10)

with

\[ Z(x) = F \sin k_x z + G \cos k_x z \]  

(11)

The application of the boundary conditions \( x = y = z = 0 \) into equations (7), (9), and (11) will be obtained by the value \( B = D = G = 0 \). The substitution of values 0 on variables \( B, D, \) and \( G \) in equations (7), (9), and (11) produces the values \( k_x, k_y, and k_z \) as follows:

\[ k_x = \frac{n_x \pi}{L} \]  

(12)

\[ k_y = \frac{n_y \pi}{L} \]  

(13)

\[ k_z = \frac{n_z \pi}{L} \]  

(14)

So that equations (7), (9), and (11) will each change to equations:

\[ X(x) = A \sin \left( \frac{n_x \pi}{L} x \right) \]  

(15)

\[ Y(y) = C \sin \left( \frac{n_y \pi}{L} y \right) \]  

(16)

\[ Z(z) = F \sin \left( \frac{n_z \pi}{L} z \right) \]  

(17)

By substituting equations (15), (16), and (17) in equation (4), the equation of the wave function for particles confined in a potential three-dimensional box is:

\[ \psi(\vec{r}) = \psi(x, y, z) = ACF \sin \left( \frac{n_x \pi}{L} x \right) \sin \left( \frac{n_y \pi}{L} y \right) \sin \left( \frac{n_z \pi}{L} z \right) \]  

(18)

The ACF value is obtained through normalization terms [10],

\[ \iiint |\psi(\vec{r}, t)|^2 dV = 1 \]  

(19)

So, that the complete solution of the particle wave function is obtained in the three-dimensional box as follows:

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

(20)

On the other, by substituting \( E_x = \frac{h^2 k_x^2}{2m}, E_y = \frac{h^2 k_y^2}{2m}, \) and \( E_z = \frac{h^2 k_z^2}{2m} \) to in equation (5) obtained from the variable \( E \)-separation method, the equation for the energy level of particles in a potential three-dimensional box is obtained as follows:

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

(21)

After obtaining wave function and energy level equations for particles in a three-dimensional box, the probability values of the particles are then formulated. Obtaining the probability particle value equation in a three-dimensional potential box is obtained by using the normalization conditions as in equation (19). In this case, it can be interpreted that the probability of finding particles in space with volume \( V \) is 100% [11]. Using equation (20), the complete solution is found for the probability of particles in a three-dimensional box as follows:

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

(22)
The final focus of this research methodology is the formulation of particle expectation value equations in three-dimensional boxes. By referring to the expectations of one-dimensional particle expectation values, namely 
\[ \langle X \rangle = \int \psi^* X \psi \, dx \]  
(23)
and substitute the particle wave function in a three-dimensional box, so that the particle expectation value equation is obtained in the three-dimensional box as follows
\[ \langle V \rangle = \frac{8}{L^3} \int \int \int \sin^2 \left( \frac{n_x \pi}{L} x \right) \sin^2 \left( \frac{n_y \pi}{L} y \right) \sin^2 \left( \frac{n_z \pi}{L} z \right) \, xyz \, dx \, dy \, dz \]  
(24)

3. Result and Discussion

The permissible energy level of a particle that is confined in a three-dimensional region depends on the price of the main quantum number of particles so that the energy value \( E \) for the particle has certain prices and must be discrete. Solving the Schrodinger equation produces a particle wave function \( \psi_{(r,t)} \) in a potential three-dimensional box which is a function of space and time variables. This wave function is then used to explain the energy level and the probability of finding particles in a potential three-dimensional box in any point interpreted by \( \psi_{(r,t)}^2 \). Using equation (21), we will obtain the calculation of the particle energy level in a potential three-dimensional box as follows,

| Quantum Number of Particles \((n_x n_y n_z)\) | Energy Level \(E\) \((10^{-16} \text{ J})\) |
|-----------------------------------------------|----------------------------------|
| 1 1 1                                         | 0.7167170769                     |
| 2 2 2                                         | 0.1791792690                     |
| 3 3 3                                         | 0.0796352307                     |
| 4 4 4                                         | 0.0447948170                     |
| 5 5 5                                         | 0.0286686830                     |

The energy level of a particle depends on its main quantum number. Based on Table 1, the calculation results show that at the base state (quantum number \( n_x = n_y = n_z = 1 \)) the particle energy will tend to be greater than the particle energy when it is in an excitation state. The higher the excitation (the longer the particles move), the less energy they have. In this case, a process called recombination will occur, which is the return of particles (electrons) in the initial state after a few moments of being excitation.

The calculation of the probability value of particles in a potential three-dimensional box in this research uses variations in the potential box width, namely \( \frac{L}{4}, \frac{L}{2}, \frac{3L}{4}, \text{and } L \) for the ground state until the fourth excitation state, with the same quantum number \((n_x = n_y = n_z)\) in each state. Using equation (22), we get the results of the calculation as follows,
Table 2. The result of mathematical data on particle probability values in a three-dimensional box

| State           | Box Width | Probability          |
|-----------------|-----------|----------------------|
| Ground (1 1 1)  | L/4       | 0,00074773143        |
|                 | L/3       | 0,125                |
|                 | L/2       | 0,206178226          |
|                 | L         | 0,206178226          |
| First excitation (2 2 2) | L/4  0,015625 |
|                 | L/3       | 0,125                |
|                 | L/2       | 0,421875             |
|                 | L         | 0,421875             |
| Second excitation (3 3 3) | L/4  0,027839769 |
|                 | L/3       | 0,125                |
|                 | L/2       | 0,338444396          |
|                 | L         | 0,338444396          |
| Third excitation (4 4 4) | L/4  0,015625 |
|                 | L/3       | 0,125                |
|                 | L/2       | 0,421875             |
|                 | L         | 0,421875             |
| Fourth excitation (5 5 5) | L/4  0,0103820417 |
|                 | L/3       | 0,125                |
|                 | L/2       | 0,477931379          |
|                 | L         | 0,477931379          |

The probability value for finding particles in a three-dimensional potential box depends on the main quantum number \((n_x, n_y, dan n_z)\), on the ground state or on the excitation state. In addition, the probability of finding a particle (electron) in a three-dimensional potential box at the position \((x, y, and z)\) is determined by the size of the potential box width. The calculation of the probability value of particles in a potential three-dimensional box can illustrate the pattern of distribution of the particle space at each point. If particles (electrons) are both in ground and excitation, either excitation in whole or in part, the probability of finding particles (electrons) in a potential box will vary.
Accordingly, with the variation in the width of the potential box, it is found that the probability of particles with a width of boxes $L_4$ and $3L_4$ has varying values in each state. For $L_2$ and $L$ particles have the same probability values in each state, namely from the ground state to the fourth excitation state. The probability of finding particles with the smallest value with potential box width $L_4$ and $3L_4$ occurs when the particle is in a ground state $(n_x = n_y = n_z = 1)$ meaning that there is very little chance of finding particles in this state. For the $L_2$ potential box width, the particle distribution pattern is obtained which is an increase in the probability value of the ground state $(n_x = n_y = n_z = 1)$ until the second excited state $(n_x = n_y = n_z = 3)$, then decreasing the probability value in the third excitation state $(n_x = n_y = n_z = 4)$ and fourth excitation state $(n_x = n_y = n_z = 5)$. For the potential box width of $3L_4$, the particle distribution pattern is obtained which is an increase in the probability value of the ground state $(n_x = n_y = n_z = 1)$ until the first excitation state $(n_x = n_y = n_z = 2)$, then decreases the probability value in the second excitation state $(n_x = n_y = n_z = 3)$, then increases the probability value again in the third excitation state $(n_x = n_y = n_z = 4)$ and fourth excitation state $(n_x = n_y = n_z = 5)$. In addition to describing the position, the particle probability value also describes the level of energy possessed by particles that are confined in a potential three-dimensional box. The energy possessed by a particle is influenced by quantum numbers also influenced by the width of the box. The wider the size of the box, the smaller the particle’s energy so that the energy level of the particles in the potential box will appear continuous.

The results of mathematical calculations in this research are supported by the plotting of images as follows,

![Figure 1](image1.png)

**Figure 1.** Probability of finding particles (electrons) in a quantum state $(n_x = n_y = n_z = 1)$ for potential box widths (a) $L_4$ (b) $L_2$ (c) $3L_4$ (d) $L$.

Figure 1 above shows that in ground conditions, the points to find particles will be found more and more in the narrower width of the box, ie at the width of the $L_4$ (there are 16 peak points) when
compared to the width of the $\frac{1}{2}L$ (there are 4 peak points), $\frac{3}{4}L$ (there are $3\frac{1}{4}$ peak points), and $L$ (there is 1 peak point).

![Figure 2](a) (b) (c) (d)

**Figure 2.** The probability of finding particles (electrons) in a quantum state $n_x = n_y = n_z = 2$ for potential box widths (a) $\frac{L}{4}$ (b) $\frac{L}{2}$ (c) $\frac{3L}{4}$ (d) $L$.

Figure 2 above shows that in the first excitation state, the points to find particles will be found more and more in the narrower width of the box, ie at the width of the $\frac{1}{4}L$ (there are 64 peak points) if compared with the width of the box $\frac{1}{2}L$ (there are 16 peak points), $\frac{3}{4}L$ (there are 9 peak points), and $L$ (there are 4 peak points). The points where particles are found in a potential box at the first excitation state are greater when compared to the ground conditions in each box width variation.
Figure 3. The probability of finding particles (electrons) in a quantum state \((n_x = n_y = n_z = 3)\) for potential box widths (a) \(\frac{L}{4}\) (b) \(\frac{L}{2}\) (c) \(\frac{3L}{4}\) (d) \(L\).

Figure 3 above shows that in the second excitation state, the points to find particles will be found more and more in the narrower width of the box, that is in the width of the \(\frac{1}{4}L\) (there are 144 peak points) if compared with the width of the box \(\frac{1}{2}L\) (there are 36 peak points), \(\frac{3}{4}L\) (there are 16 peak points), and \(L\) (there are 9 peak points). The points found in particles in a potential box in the second excitation state are greater when compared to the ground state and the first excitation state in each box width variation.

Figure 4. The probability of finding particles (electrons) in a quantum state \((n_x = n_y = n_z = 4)\) for potential box widths (a) \(\frac{L}{4}\) (b) \(\frac{L}{2}\) (c) \(\frac{3L}{4}\) (d) \(L\).

Figure 4 above shows that in the third excitation state, the points to find particles will be found more and more in the narrower width of the box, that is in the width of the \(\frac{1}{4}L\) (there are 256 peak points) if compared with the width of the box \(\frac{1}{2}L\) (there are 64 peak points), \(\frac{3}{4}L\) (there are 36 peak points), and \(L\) (there are 16 peak points). The points found in particles in a potential box in the third
excitation state are more than those in the ground state or in the first and second excitation states in each box width variation.

Figure 5. The probability of finding particles (electrons) in a quantum state \( n_x = n_y = n_z = 5 \) for potential box widths (a) \( \frac{L}{4} \) (b) \( \frac{L}{2} \) (c) \( \frac{3L}{4} \) (d) \( L \).

Figure 5 above shows that in the fourth excitation state, the points to find particles will be found more and more in the narrower width of the box, ie at the width of the \( \frac{1}{4}L \) (there are 400 peak points) if compared to the width of the box \( \frac{1}{2}L \) (there are 100 peak points), \( \frac{3}{4}L \) (there are 49 peak points), and \( L \) (there are 25 peak points). The points where particles are found in a potential box in the fourth excitation state are greater than those in the ground state or in the first, second, and third excitation states in each box width variation.

The graphs presented in each of the images above describe the probability of finding particles (electrons) in a potential three-dimensional box in each state, from the ground state to the fourth excitation state, using the variation of the potential box width for each quantum state. The narrower the size of the potential side of the box, the smaller the probability value is obtained, but the points to find the presence of particles in the potential box will increase, where this corresponds to the mathematical calculations in table 2 and the graph projection in figure 1-5.

The calculation of the expectation value of particles in a potential three-dimensional box in this research uses variations in the potential box width, namely \( \frac{L}{4} \), \( \frac{L}{2} \), \( \frac{3L}{4} \), and \( L \) for the ground state until the fourth excitation state, with the same quantum number \( n_x = n_y = n_z \) in each state. Using equation (24), we get the results of the calculation as follows.

Table 3. The result of mathematical data on particle expectation values in a three-dimensional box

| State   | Box Width | Expectation Values \( (L^3) \) |
|---------|-----------|--------------------------------|
| Ground  | \( \frac{L}{4} \) | 0.00000473916085               |
| State         | Box Width | Expectation Values($L^3$) |
|--------------|-----------|---------------------------|
| (1 1 1)      | $\frac{L}{2}$ | 0.00542505614             |
|              | $\frac{3L}{4}$ | 0.0773266074             |
|              | $L$         | 0.125                     |
| First excitation | $\frac{L}{4}$ | 0.0000847665027         |
| (2 2 2)      | $\frac{L}{2}$ | 0.001953125              |
|              | $\frac{3L}{4}$ | 0.0253935181             |
|              | $L$         | 0.125                     |
| Second excitation | $\frac{L}{4}$ | 0.000126160866         |
| (3 3 3)      | $\frac{L}{2}$ | 0.00222933491             |
|              | $\frac{3L}{4}$ | 0.0145729881             |
|              | $L$         | 0.125                     |
| Third excitation | $\frac{L}{4}$ | 0.0000305175781        |
| (4 4 4)      | $\frac{L}{2}$ | 0.001953125              |
|              | $\frac{3L}{4}$ | 0.0222473145             |
|              | $L$         | 0.125                     |
| Fourth excitation | $\frac{L}{4}$ | 0.0000143532591      |
| (5 5 5)      | $\frac{L}{2}$ | 0.00204976137             |
|              | $\frac{3L}{4}$ | 0.0286946576             |
|              | $L$         | 0.125                     |

The expectation value of particles in the $\frac{L}{4}$ sized three-dimensional box is found that from the ground state to the second excitation state the value increases, but from the second excitation state to the fourth excitation state the value decreases. The expectation value with width $\frac{L}{4}$ is proportional to the probability. The expectation value of particles in the $\frac{L}{2}$ sized three-dimensional box is found that from the ground state to the fourth excitation state the value is fluctuating, where this does not correspond to the probability of equal value in all state. The expectation value of particles in a three-dimensional box measuring $\frac{3L}{4}$ is found that from the ground state to the second excitation state the value decreases, but from the second excitation state to the fourth excitation state the value increases. The expectation value with a width of $\frac{3L}{4}$ is inversely proportional to the probability. The expectation value of particles in
a three-dimensional box of size $L$ is found that from the ground state to the fourth excitation state the value is the same, where this corresponds to the probability that is equal in all state.

4. Conclusion
The results of the research and discussion, it can be concluded that the probability of finding particles (electrons) in a three-dimensional box is determined by the size of the box so that a probability (probability per unit volume) is found to find the particles ($x, y, \text{and} z$), with thus it can be calculated and illustrated the pattern of the spread of these particles at each point. In addition, the probability of finding particles and energy levels in three-dimensional squares depends on quantum numbers ($n_x = n_y = n_z$). In this research taken until the fourth undegenerated excitation state means that the quantum number of particles is fully excitation, if the particle is in a state excitation then the probability of finding particles (electrons) in a box also varies depending on certain excitation states. Based on the calculation of the expectation value it is found that the box size to find the most stable particles in the ground state until the fourth excitation state is at the width $L_4$ and $L$. Suggestions that can be offered to the next researcher are calculation of the probability values and expectation values by controlling potential box widths that are more than $L$, variations on quantum number values ($n_x \neq n_y \neq n_z, n_x = n_y \neq n_z, \text{and} n_x \neq n_y = n_z$), or it could be by adding the value of the quantum number $\geq 5$.

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