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# *Degeneracy and Symmetry of the Infinite Potential Well*

**Yuanbei Sun**

*Shandong Experimental High School, Jinan, China*
*874493121@qq.com*

***Abstract:*** This paper solves the wavefunctions and energy level formulas of two types of three-dimensional infinite deep cubic potential wells and three-dimensional infinite deep spherical potential wells, and studies their degeneracy to elucidate how symmetry governs energy level degeneracy in quantum systems. For the cubic potential well, the potential energy inside the cube is zero, and outside the cube is infinite. Solving the Schrödinger equation shows that the energy is determined by the total of the squares of three quantum numbers $(n_x, n_y, n_z)$. Degeneracy occurs when different combinations of quantum numbers produce the same sum of squares, which reflects cubic symmetry, i.e., the equivalence of the x, y, and z directions, such that permuted states are physically identical. For the spherical potential well, the potential energy inside the sphere is zero, and outside the sphere is infinite. The wavefunction can be devided into angular and radial parts. The energy depends on the radial quantum number $n$ and the angular momentum quantum number $l$, and degeneracy arises from the magnetic quantum number $m$, which ranges from $-l$ to $l$. Since the potential energy of the spherical potential well is independent of direction, it has spherical symmetry, which leads to degeneracy of magnitude $2l + 1$-fold. To summarize, the degeneracy of the cubic potential well originates from its cubic symmetry, while that of the spherical potential well originates from its spherical symmetry. This highlights the central role of symmetry in quantum energy level degeneracy.

***Keywords:*** Three-dimensional infinite cubic potential well, Three-dimensional infinite spherical potential well, Energy level degeneracy, Symmetry-governed degeneracy, Schrödinger equation

## 1. Introduction

As a fundamental theory describing the microscopic world, quantum mechanics depicts the energy level structure and state properties of quantum systems through the solutions of the Schrödinger equation. [1] [2] [3] Among numerous quantum system models, the infinite square potential well stands out as one of the most classic examples for understanding quantum bound states due to its simple form and clear physical imagery.

Extending the infinite square well to multiple dimensions transforms it into a powerful tool for exploring the interaction between degeneracy and symmetry. For instance, in a three-dimensional infinite cubic well, the three coordinates can be interchanged with each other without affecting the

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potential energy result, thus cubic symmetry leads to degeneracy. In a spherical well, the potential energy is independent of direction, thus spherical symmetry leads to degeneracy.

Multidimensional infinite square wells not only deepen the understanding of the spatiotemporal distribution of quantum states but also provide an ideal platform for investigating the relationship between degeneracy and symmetry in quantum systems.

## 2. Model

### 2.1. Three-dimensional cubic infinite square potential well

The potential energy function of a three-dimensional infinite square potential well with length L is defined as:

$$V(x,y,z) = \begin{cases} 0 & \text{if } 0 < x,y,z < L \\ \infty & \text{if } x,y,z \le 0 \text{ or } x,y,z \ge L \end{cases} \tag{1}$$

Let the wavefunction be $\psi(x,y,z)$, for a particle with mass m, the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z) \tag{2}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Outside the potential well, since the potential energy is positive infinity and the energy must remain finite, therefore

$$\psi(x,y,z) = 0 \quad \text{when } x,y,z \le 0, \text{ or } x,y,z \ge L \tag{3}$$

Inside the potential well, the potential energy is 0, therefore the Schrödinger equation reduces to

$$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi(x,y,z) = E\psi(x,y,z) \tag{4}$$

We assume that our wavefunction is the product of three independent functions X(x), Y(y) and Z(z):

$$\psi(x,y,z) = X(x)Y(y)Z(z) \tag{5}$$

Then, the Schrödinger equation can be presented as

$$-\frac{\hbar^2}{2m}(YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 Z}{\partial z^2}) = EXYZ \tag{6}$$

Therefore,

$$E_x = -\frac{\hbar^2}{2m}\frac{1}{X}\frac{\partial^2 X}{\partial x^2} \quad , \tag{7}$$

$$E_y = -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} \quad , \tag{8}$$

$$E_z = -\frac{\hbar^2}{2m}\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} \tag{9}$$

$$E = E_x + E_y + E_z \tag{10}$$

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In this way, through separating variables, we have transformed the three-dimensional problem into a one-dimensional problem.

Recall the solution of one-dimensional infinite potential well:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad 0 \le x \le L \tag{11}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \tag{12}$$

where $n \in Z^+$.

Therefore, the expressions of the wavefunction and energy in three dimension are

$$\psi_{n_x,n_y,n_z}(x,y,z) = (\frac{2}{L})^{3/2} \sin\left(\frac{n_x\pi x}{L}\right) \sin\left(\frac{n_y\pi y}{L}\right) \sin\left(\frac{n_z\pi z}{L}\right) \quad 0 \le x,y,z \le L \tag{13}$$

$$E_{n_x,n_y,n_z} = E_{n_x} + E_{n_y} + E_{n_z} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \tag{14}$$

where $n_x, n_y, n_z \in Z^+$.

It can be seen from equations (2.1..13) and (2.1..14) that the energy of the particles is determined by the combination of $n_x$,$n_y$ and $n_z$, while the state is determined by the permutation of them. Therefore, the energy and state of the particles can be given by the permutation $(n_x, n_y, n_z)$. At this point, if different sets of the quantum numbers $(n_x, n_y, n_z)$ correspond to the same sum of squares, then the energy level is degenerate.

More generally speaking, we can denote

$$n_x^2 + n_y^2 + n_z^2 = N \tag{15}$$

$$\frac{\pi^2\hbar^2}{2mL^2} = \epsilon \tag{16}$$

$$E_{n_xn_yn_z} = N\epsilon \tag{17}$$

In this way, the problem becomes: given the constant N, find all positive integer solutions that satisfy equation (2.1..15). When the equation has a unique solution, the energy level is non-degenerate; when the equation has multiple sets of solutions, the energy level is degenerate, where the number of solution sets corresponds to the degeneracy of energy level N. [4]

For example,

– if a system has energy $E = 6\epsilon$, the combination of its quantum numbers is 1,1,2, so the permutation of its quantum numbers could be (1,1,2), (1,2,1) or (2,1,1). The possible wavefunctions are:

$$\psi_{1,1,2} = (\frac{2}{L})^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right) \tag{18}$$

$$\psi_{1,2,1} = (\frac{2}{L})^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \tag{19}$$

$$\psi_{2,1,1} = (\frac{2}{L})^{3/2} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \tag{20}$$

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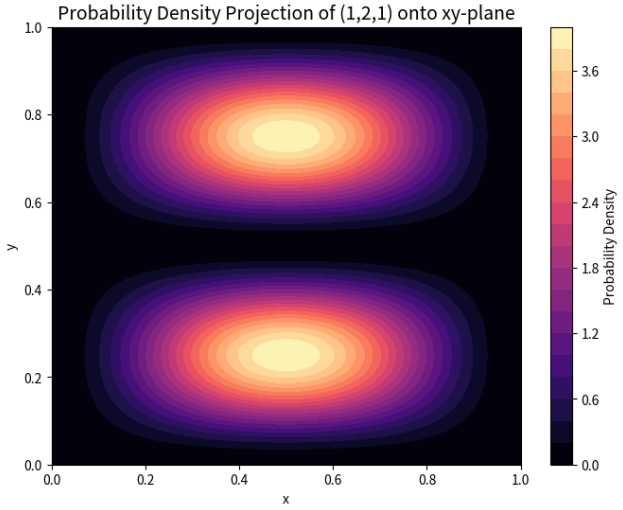


Figure 1: Probability Density Projection of (1,2,1) onto xy-plane

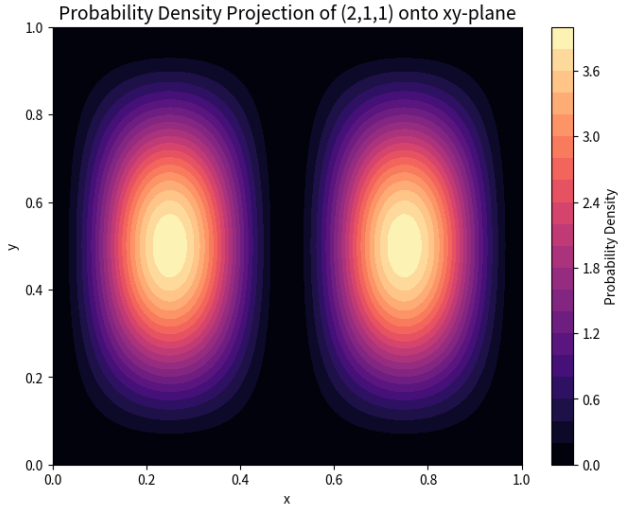


Figure 2: Probability Density Projection of (2,1,1) onto xy-plane

Therefore, this energy is degenerate, with a degeneracy of 3.

The two figures below shows the projections along the x and y directions of two of the cases above.

Figure 1 is the projection of the (1,2,1) wavefunction, and Figure 2 is the projection of the (2,1,1) wavefunction. Consequently, these wavefunctions exhibit xy exchange symmetry on planes where z remains constant.

– if a system has energy $E = 12\epsilon$, the permutation of its quantum numbers can only be (2,2,2):

$$\psi_{2,2,2} = (\frac{2}{L})^{3/2} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right) \tag{21}$$

Therefore, this energy is non-degenerate;

– if a system has energy $E = 14\epsilon$, the combination of its quantum numbers is 1,2,3, so the permutation of its quantum numbers could be (1,2,3), (1,3,2), (2,1,3), (2,3,1), (3,1,2) and (3,2,1). Therefore, this energy is degenerate, with a degeneracy of 6;

– if a system has energy $E = 27\epsilon$, the combination of its quantum numbers could either be 1,1,5 or 3,3,3. Among them, 1,1,5 has 3 different permutations, while 3,3,3 has only 1. Therefore, this energy is degenerate, with a degeneracy of 4.

Notably, here we can see that the degeneracy of energy $E_{n_x,n_y,n_z} = (\pi^2\hbar^2)/(2mL^2)(n_x^2+n_y^2+n_z^2)$ is not necessarily identical to the quantity of different permutations of $\{n_x, n_y, n_z\}$ , but depends on the specific circumstances.

Looking back to the expression (2.1..1), since the potential energy expression is exactly the same for the three orthogonal axes $x$, $y$, and $z$ (the potential energy equals zero when the position is less than or equal to $L$, and positive infinity when it is greater than $L$), these three coordinate axes can be interchanged with each other without affecting the potential energy result. Therefore, they are equivalent in some sense, meaning that the potential energy has cubic symmetry. Due to the symmetry of the potential energy, the solutions must also possess such symmetry, hence the degeneracy caused by symmetry.

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## 2.2. Three-dimensional spherical infinite square potential well

The potential energy function of a three-dimensional infinite spherical square potential well with radius r is defined as:

$$V(r) = \begin{cases} 0 & \text{if } 0 < r < L \\ \infty & \text{if } r \geq L \end{cases} \tag{1}$$

Let the wavefunction be $\psi(r, \theta, \phi)$, for a particle with mass m, the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) + V(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{2}$$

with the Laplacian expressed in spherical coordinates taking the form

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{3}$$

Similarly, the wavefunction when $r \geq L$ is always equal to 0. When $r < 0$, the equation becomes

$$-\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{4}$$

The wavefunction is able to be separated into radial and angular sections:

$$\psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi) \tag{5}$$

Substituting it into the Schrödinger equation, the equation's radial component becomes

$$-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\hbar^2 l(l+1)}{2mr^2}R = ER \tag{6}$$

and the angular part of the equation is

$$\hat{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi) \tag{7}$$

where $\hat{L}^2$ is the angular momentum squared operator, $l = 0, 1, 2, \ldots$ is the angular momentum quantum number, $m = -l, -l+1, \ldots, l$ is the magnetic quantum number and $Y_{lm}$ is the spherical harmonic function.

Defining $u(r) = rR(r)$, the radial part of the equation (2.2..6) becomes

$$-\frac{\hbar^2}{2m}u'' + \left[\frac{\hbar^2 l(l+1)}{2mr^2}\right]u = Eu \tag{8}$$

Here we have two boundary conditions:

- When $r = 0$, $u(0) = 0$ (ensures the wavefunction is finite);
- When $r = a$, $u(a) = 0$ (wavefunction equals to zero outside the potential well).

The equation resembles a one-dimensional infinite potential well, but the effective potential includes the centrifugal potential $(\hbar^2 l(l+1))/(2mr^2)$.

The radial solution is described by the spherical Bessel function $j_l(kr)$, which satisfies $u(a) = 0$, i.e., $j_l(ka) = 0$.

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Let $ka = \alpha_{nl}$, where $\alpha_{nl}$ is the nth positive root of the spherical Bessel function $j_l$, $n = 1, 2, 3, \cdots$ is the radial quantum number, then the energy eigenvalue is:

$$E_{nl} = \frac{\hbar^2 \alpha_{nl}^2}{2mL^2} \tag{9}$$

Total wavefunction:

$$\psi_{nlm}(r, \theta, \phi) = N_{nl} j_l \left( \frac{\alpha_{nl} r}{L} \right) Y_{lm}(\theta, \phi) \tag{10}$$

with $N_{nl}$ representing the normalization constant.

From the expression of energy (2.2..9), we can see that the energy is proportional to $a_{nl}$, which is obviously determined by the values of $n$ and $l$. Therefore, for a system with given values of $n$ and $l$, the energy eigenvalue $E$ is uniquely determined.

At this point, for this definite energy value, the only variable part of the wavefunction lies in its angular part: the magnetic quantum number $m$. Therefore, the quantity of all possible states, that is, the degeneracy of this energy, is equal to the range of values of $m$, which is $2l + 1$ values ranging from $-l$ to $l$.

$$\text{Degeneracy} = 2l + 1 \tag{11}$$

## 3. Results and Discussion

### 3.1. Solutions

1. For three-dimensional cubical infinite square potential well:
   The energy eigenvalues are determined by the total obtained from squaring the quantum numbers:

$$E_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2mL^2} \left( n_x^2 + n_y^2 + n_z^2 \right) \equiv N\epsilon \tag{1}$$

   where $N = n_x^2 + n_y^2 + n_z^2 (n_x, n_y, n_z \in \mathbb{Z}^+)$ and $\epsilon = (\pi^2 \hbar^2)/(2mL^2)$.
   Degeneracy arises from distinct sets of $\{n_x, n_y, n_z\}$ yielding the same N.
2. For three-dimensional spherical infinite square potential well:
   Energy depends on radial and angular quantum numbers:

$$E_{nl} = \frac{\hbar^2 \alpha_{nl}^2}{2mL^2} \tag{2}$$

   where $\alpha_{nl}$ is the n-th root of the spherical Bessel function $j_l(x)$.
   Degeneracy is determined by the magnetic quantum number $m(m = -l, -l + 1, \ldots, l)$, yielding $2l + 1$-fold degeneracy.

### 3.2. The Relationship Between Degeneracy and Symmetry

In both the three-dimensional infinite cubic potential well and the spherical potential well, the degeneracy arises from symmetry. [5]

1. For cubical well: degeneracy is dominated by cubic symmetry
   The high symmetry of the cubic potential well is reflected in the "equivalence" of the x, y, and z directions, due to the exactly identical boundary conditions for these three directions of the potential well. This symmetry leads to the "commutativity" of the quantum numbers $n_x, n_y, n_z$: exchanging any two quantum numbers will not change the system's physical state. Thus, the energies of the corresponding quantum states must be identical, which therefore leads to degeneracy.

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2. For spherical well: degeneracy is dominated by spherical symmetry
   The spherical potential well exhibits spherical symmetry, meaning its potential depends only on radial distance r and is independent of angles $\theta$ and $\phi$. This symmetry ensures that quantum states with the same radial part $R(r)$ (that is, identical n and l) have the same energy. Additionally, in the angular wavefunction $Y_{lm}$, m denotes the angular momentum projection onto the z-axis. Due to the lack of a "preferred direction" in a spherically symmetric potential, states with different $m$ are energetically indistinguishable, leading to a degeneracy of $2l + 1$. Thus, the system's energy depends solely on the magnitude of angular momentum quantum number $l$.

## 4. Conclusion

In summary, this paper analyzes the energy level structures and degeneracies of two types of three-dimensional infinite square wells (cubic and spherical), revealing the central role of symmetry in the energy degeneracy of quantum states.

For cubic well, energy levels are decided by the sum of the squares of quantum numbers $N = n_x^2 + n_y^2 + n_z^2$, and degeneracy arises from the equivalence of the x, y, and z directions. For spherical well, energy levels are determined by the radial quantum number $n$ the angular momentum quantum number $l$. Degeneracy is entirely dominated by the possible values taken by the magnetic quantum number $m$ (i.e., $2l + 1$), which directly results from spherical symmetry, where no direction is preferred, making all m-states energetically equivalent.

These results deepen the understanding of quantum confinement in symmetric potentials and provide a foundation for studying more complex systems (e.g., anisotropic wells or those with external fields).

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