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Periodicity of the Probability Distribution of a Particle in a Box

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ABSTRACT

We consider a particle in a two-dimensional infinite potential square well in states that are superpositions of either two or three energy eigenstates. These have probability distributions that are periodic in time. We compute the periods in both cases and simulate the time dependence of the probability distributions.

Keywords: *Physics, Quantum Mechanics, Probability Distributions, Eigenstates, Simulation, Particle in A Box*

1. INTRODUCTION

In quantum mechanics, the time-dependent solution to the Schrodinger equation gives the wavefunction $\psi(\vec{r},t)$. Because this equation is separable into spatial and temporal parts, the time dependence of $\psi(\vec{r},t)$ (for energy eigenfunctions) is a simple phase. Therefore, in this case, the probability distribution function (PDF) $|\psi(\vec{r},t)|^2$ is time-independent. On the other hand, when the wavefunction is a superposition of different energy eigenstates, the PDF is time-dependent. In these cases, the PDF is also periodic[1]. In this paper, we obtain the periods of the PDF for different superpositions of two or three eigenstates explicitly. For superpositions of more than three eigenstates, the periods can be obtained by similar methods used for the three-eigenstate case. We will show the time dependence of the PDF in the next section.

2. METHODS

A simple example that demonstrates the time dependence of the PDF is a particle in a two-dimensional infinite potential well (box). For simplicity, we consider a square well with $L_x = L_y = L$ where L_x and L_y are the dimensions of the box.

The solution to the Schrodinger's equation for a particle in such a box is (See appendix A.)

$$\psi(x,y,t) = \frac{2}{L}\cdot\sin\left(\frac{n\pi x}{L}\right)\cdot\sin\left(\frac{m\pi y}{L}\right)\cdot e^{\pi i E(n,m)\cdot\frac{t}{\hbar}} \tag{1}$$

where n and m are quantum numbers that determine the momenta of the particle in the x and y directions, respectively. The wavefunctions in eq. (1) are energy eigenfunctions with energies

$$E(n,m) = \frac{\hbar^2}{2ML^2}(n^2+m^2) \tag{2}$$

where M is the mass of the particle. As we mentioned above, a wavefunction that is an energy eigenfunction has a simple phase as in eq. (1). Therefore, the PDF $|\psi(x,y,t)|^2$ is time independent.

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[1] In addition, periodicity requires that the dimensions of the box satisfy $L_y^2 = kL_x^2$ where k is rational. See the discussion at end of section 3.

The simplest wavefunction with a time dependent PDF is given by a superposition of two energy eigenfunctions $\psi = \psi_1 + \psi_2$ where

$$\psi_1(x,y,t) = \frac{2}{L} \cdot \sin\left(\frac{n_1 \pi x}{L}\right) \cdot \sin\left(\frac{m_1 \pi y}{L}\right) \cdot e^{\pi i E(n_1,m_1) \cdot \frac{t}{\hbar}} \tag{3}$$

$$\psi_2(x,y,t) = \frac{2}{L} \cdot \sin\left(\frac{n_2 \pi x}{L}\right) \cdot \sin\left(\frac{m_2 \pi y}{L}\right) \cdot e^{\pi i E(n_2,m_2) \cdot \frac{t}{\hbar}} \tag{4}$$

The next simplest wavefunction with a time-dependent PDF is given by the superposition of three eigenfunctions, $\psi = \psi_1 + \psi_2 + \psi_3$ where

$$\psi_1(x,y,t) = \frac{2}{L} \cdot \sin\left(\frac{n_1 \pi x}{L}\right) \cdot \sin\left(\frac{m_1 \pi y}{L}\right) \cdot e^{\pi i E(n_1,m_1) \cdot \frac{t}{\hbar}} \tag{5}$$

$$\psi_2(x,y,t) = \frac{2}{L} \cdot \sin\left(\frac{n_2 \pi x}{L}\right) \cdot \sin\left(\frac{m_2 \pi y}{L}\right) \cdot e^{\pi i E(n_2,m_2) \cdot \frac{t}{\hbar}} \tag{6}$$

$$\psi_3(x,y,t) = \frac{2}{L} \cdot \sin\left(\frac{n_3 \pi x}{L}\right) \cdot \sin\left(\frac{m_3 \pi y}{L}\right) \cdot e^{\pi i E(n_3,m_3) \cdot \frac{t}{\hbar}} \tag{7}$$

In the next section, we will compute the periods of the two cases we considered above.

The period of the probability distribution

In the case where the wavefunction is the sum of two energy eigenfunctions, the PDF is

$$|\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + 2\cos\left(\frac{\pi \Delta E}{\hbar} t\right) |\psi_1||\psi_2| \tag{8}$$

We see that the PDF has a time dependence that is given by $\cos\left(\frac{\pi \Delta E t}{\hbar}\right)$. Therefore, the PDF is not only time dependent but also periodic. This period is given by

$$T = \frac{2\hbar}{\Delta E} = \frac{ML^2}{\hbar\left((n_2^2 - n_1^2) + (m_2^2 - m_1^2)\right)} \tag{9}$$

where (n_1, m_1) and (n_2, m_2) correspond to ψ_1 and ψ_2 respectively.

In the case where the wavefunction is the sum of three energy eigenfunctions, the PDF is

$$\begin{aligned} |\psi|^2 \; \& = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + 2\cos(\omega_{1,2} t) |\psi_1||\psi_2| + 2\cos(\omega_{1,3} t) |\psi_1||\psi_3| \\ + 2\cos(\omega_{2,3} t) |\psi_2||\psi_3| \end{aligned} \tag{10}$$

where $\omega_{i,j} = \frac{\pi(E_i - E_j)}{\hbar}$ for $i \neq j$ and $i, j \in \{1,2,3\}$ and where $E_i = E(n_i, m_i)$.

In this case, the time dependence of the PDF is more complicated i.e., it is a sum of three cosine functions with different periods, which are

$$T_1 = \frac{2\hbar}{\Delta E_{1,2}} \qquad T_2 = \frac{2\hbar}{\Delta E_{1,3}} \qquad T_3 = \frac{2\hbar}{\Delta E_{2,3}} \tag{11}$$

Substituting E_1, E_2, and E_3, we get for the periods of the cosine functions:

$$T_1 = \frac{4ML^2}{\hbar\left((n_2^2 - n_1^2) + (m_2^2 - m_1^2)\right)} = \frac{4ML^2}{\hbar a} \tag{12}$$

$$T_2 = \frac{4ML^2}{\hbar\left((n_3^2 - n_1^2) + (m_3^2 - m_1^2)\right)} = \frac{4ML^2}{\hbar b} \tag{13}$$

$$T_3 = \frac{4ML^2}{\hbar\left((n_3^2 - n_2^2) + (m_3^2 - m_2^2)\right)} = \frac{4ML^2}{\hbar c} \tag{14}$$

where a, b, c are integers defined by

$$a = (n_2^2 - n_1^2) + (m_2^2 - m_1^2) \tag{15}$$

$$b = (n_3^2 - n_1^2) + (m_3^2 - m_1^2) \tag{16}$$

$$c = (n_3^2 - n_2^2) + (m_3^2 - m_2^2) \tag{17}$$

Let the period of this PDF be T. In order for the PDF to be periodic, T has to be integer multiples of T_1, T_2, T_3. If a, b, c defined above have $gcd(a, b, c) = 1$, then

$$T = \frac{4ML^2}{\hbar} = aT_1 = bT_2 = cT_3 \tag{18}$$

However, when a, b, c have a greatest common divisor $gcd(a, b, c) \neq 1$, the shortest period becomes

$$T = \frac{4ML^2}{\hbar \cdot gcd(a, b, c)} \tag{19}$$

Above, we considered, for simplicity, a square well with $L_x = L_y$. If $L_x \neq L_y$, then whether the PDF has a period or not depends on the relation between L_x^2 and L_y^2.

$$T_1 = \frac{4ML_x^2L_y^2}{\hbar\left((n_2^2 - n_1^2)L_x^2 + (m_2^2 - m_1^2)L_y^2\right)} \tag{20}$$

with similar modifications to T_2 and T_3 given by eqs. (13) and (14).
When $L_y^2 = \frac{p}{q}L_x^2$, where $p, q \in N$,

$$T_1 = \frac{4ML_xL_{y\sqrt{pq}}}{\hbar\left((n_2^2 - n_1^2)p + (m_2^2 - m_1^2)q\right)} \tag{21}$$

$$T_2 = \frac{4ML_xL_{y\sqrt{pq}}}{\hbar\left((n_3^2 - n_1^2)q + (m_3^2 - m_1^2)p\right)} \tag{22}$$

$$T_3 = \frac{4ML_xL_{y\sqrt{pq}}}{\hbar\left((n_3^2 - n_2^2)q + (m_3^2 - m_2^2)p\right)} \tag{23}$$

From $aT_1 = bT_2$, we have

$$bL_x^2\frac{p}{q}(n_1^2 - n_2^2) + bL_x^2(m_1^2 - m_2^2) = aL_x^2\frac{p}{q}(n_1^2 - n_3^2) + aL_x^2(m_1^2 - m_3^2) \tag{24}$$

and

$$a\left(p(n_1^2 - n_3^2) + q(m_1^2 - m_3^2)\right) = b\left(p(n_1^2 - n_2^2) + q(m_1^2 - m_2^2)\right) \tag{25}$$

There is always a period which corresponds to the simplest solution with $a = p(n_1^2 - n_2^2) + q(m_1^2 - m_2^2)$ and $b = p(n_1^2 - n_3^2) + q(m_1^2 - m_3^2)$. Note that this does not necessarily give the shortest period, since $gcd(a, b)$ is not guaranteed to be 1. From $T = aT_1$, we get

$$T_{max} = \frac{4ML_x^2p}{\hbar} = \frac{4ML_xL_{y\sqrt{pq}}}{\hbar} = aT_1 = bT_2 = cT_3 \tag{26}$$

If a, b, c have a common factor r, then the period of the function will be $\frac{T_{max}}{r}$. So, when a, b, c has a gcd greater than one, the smallest period of the function will be

$$T = \frac{T_{max}}{gcd(a, b, c)} \tag{27}$$

The period given above seems to be independent of the parameters n_i, m_i which determine the energies of the eigenfunctions that form the superposition. However this is incorrect since a, b, c depend upon n_i, m_i as given by eq.(15-17).

If $L_y^2 = kL_x^2$ where k is irrational, then the PDF is not periodic. In order to show this, we first assume that the PDF is periodic even when k is irrational. This implies again that $aT_1 = bT_2$ which can be written as

$$bk(n_1^2 - n_2^2) - ak(n_1^2 - n_3^2) = a(m_1^2 - m_3^2) - b(m_1^2 - m_2^2) \tag{28}$$

which gives

$$k = \frac{a(m_1^2 - m_3^2) - b(m_1^2 - m_2^2)}{b(n_1^2 - n_2^2) - a(n_1^2 - n_3^2)} \tag{29}$$

By assumption, k is irrational whereas the right-hand side, must be rational since $a, b, m_1, m_2, m_3, n_1, n_2, n_3$ are all integers. Therefore, when k is irrational, our original assumption was wrong i.e., the PDF is not periodic. Note that if k is an arbitrary real number, then there will almost never be a period.

When the wavefunction is a superposition of $n > 3$ energy eigenstates, the PDF will have $n(n-1)/2$ cosines that are functions of time with different periods. The derivation of the overall periods and the discussion of the case $L_y^2 = kL_x^2$ are identical to the three-eigenstate case.

3. RESULTS AND DISCUSSION

We simulate the PDF as a function of time and show that it is periodic. We take the particle in the box to be an electron which fixes $M = 9.109 \cdot 10^{-31}$ kg. We set the side length of the box L to be $L = 10^{-9}\ m$. We divide the LxL box into cells of size $\frac{L}{100}$x $\frac{L}{100}$. In our simulation, we compute the values of the PDF in time increments of

$$\Delta t = \frac{4M}{\hbar}\left(\frac{1}{L_x^2} + \frac{1}{L_y^2}\right) \quad (30)$$

and generate the simulation.

For the two-eigenstate case of this simulation, there are four input parameters: n_1, n_2, m_1, and m_2. We compute E_1 and E_2 using these parameters. Then we define two functions $\sin_1(x,y) = \sin\left(\frac{\pi n_1 x}{L}\right)\sin\left(\frac{\pi m_1 y}{L}\right)$ and $\sin_2(x,y) = \sin\left(\frac{\pi n_2 x}{L}\right)\sin\left(\frac{\pi m_2 y}{L}\right)$. This allows us to construct the time dependent and the time independent parts of $|\psi|^2$ as $\psi_{const} = \frac{2}{L^2}(\sin_1^2(x,y)\sin_2^2(x,y))$ and $\psi_t = \frac{4}{L^2}\sin_1(x,y)\sin_2(x,y)\cos\left(\frac{\pi(E_1-E_2)t}{\hbar}\right)$. We compute the values $\psi_t + \psi_{const}$ in each cell in the time increments given above and create its 3D simulation.

For the case with three eigenstates, the parameters are identical to the two-eigenstate case and the setup and graphing are similar. The only differences are the additional parameters n_3 and m_3. These appear in another sin function $\sin_3(x,y) = \sin\left(\frac{\pi n_3 x}{L}\right)\sin\left(\frac{\pi m_3 y}{L}\right)$. We define the portion of eq. (10) that has no sin component as ψ_{const} which is the constant term, with the rest being the time-dependent part ψ_t.

We provide four simulations of the two eigenfunction case and six simulations of the three eigenstate case. In detail, we simulated the cases with the parameters. For the four simulations with two eigenstates, (n_1, m_1, n_2, m_2) take the values (1,1,1,2), (1,2,1,3), (1,2,2,2), (1,2,3,1). For the six simulations with three eigenstates, $(n_1, m_1, n_2, m_2, n_3, m_3)$ take the values (1,1,1,2,1,3), (1,1,1,2,3,1), (1,1,2,3,1,3), (1,2,5,5,3,1), (4,1,3,2,1,3), and (4,5,1,2,3,1).

These simulations can be seen here. Each simulation takes a time length of two periods. After one period, we briefly stop the time evolution in order to show the periodicity of the PDF. We observe that some PDFs change quite fast, whereas others change much slower.

A visual representation is shown in Figure 1 – 4 in below.

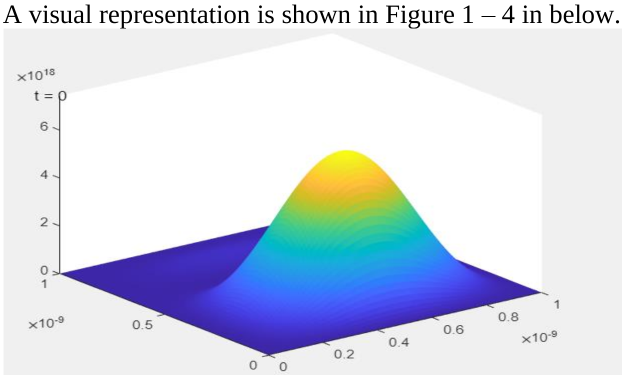

Figure 1: $(n_1, m_1) = (1,1)$ and $(n_2, m_2) = (1,2)$ at time t = 0.

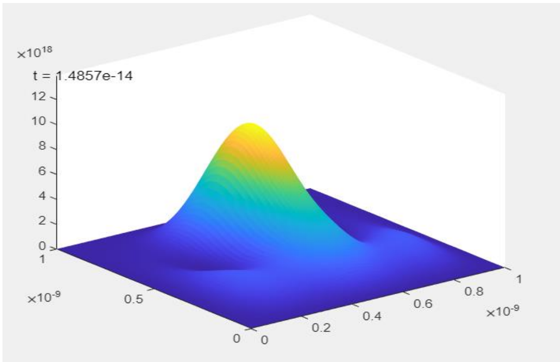

Figure 2: $(n_1, m_1) = (1,1)$, $(n_2, m_2) = (1,2)$, and $(n_3, m_3) = (3,1)$ at time $t = 1.4857 \cdot 10^{-14}$ s.

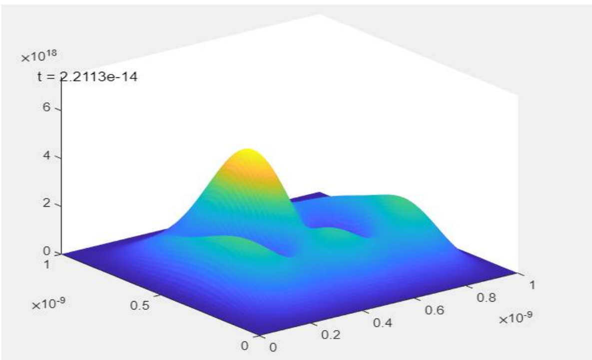

Figure 3: $(n_1, m_1) = (1,2)$ and $(n_2, m_2) = (3,1)$ at time $t = 2.2113 \cdot 10^{-14}$ s

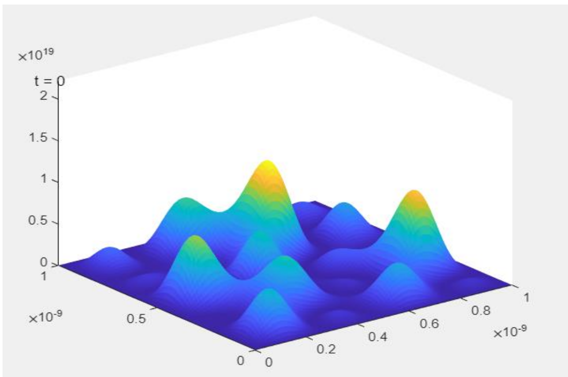

Figure 4: $(n_1, m_1) = (4,5)$, $(n_2, m_2) = (1,2)$, and $(n_3, m_3) = (3,1)$ at time t = 0.

4. CONCLUSION

We found the time-dependent PDFs for wavefunctions that are superpositions of two or three energy eigenfunctions. In both cases, these PDFs contain a constant term and a time dependent term where the time dependence is given by a cosine function. As a result, the PDFs are periodic when $\frac{L_x}{L_y}$ is rational. We simulated a number of PDFs with different parameters. These are also shown on YouTube here. The simulations demonstrate the periodicity of the PDFs. Our results can easily be generalized to the superpositions of $n > 3$ eigenstates. In those cases, the time-dependent behavior of the PDF is very similar to the three-eigenstate case.

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6. REFERENCES

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