A Statistical Approach to an Infinite Potential Well

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1 Introduction

In classical mechanics, Newton's Second Law describes the time evolution of a particle. Analogously, the Schrodinger Equation,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi,$$

describes the time evolution of a particle in Quantum Mechanics. The function Ψ is referred to as the wavefunction of the particle and it gives information about the state of the particle.

In this paper we will study the solutions of the Schrodinger Equation for a particle in an infinite potential well. In particular, we will calculate statistically significant quantities such as the expected value and standard deviations of the particles position and momentum. Lastly, we will discuss the application of these quantities to Heisenberg's Uncertainty Principle.

2 Infinite Potential Well

Consider an electron on a one dimensional segment of width 8 nm. If the electron is free to move along this line and is forced to stay on this line by an infinite force present at each end of the line segment, then the electron is said to be in an infinite potential well.

Let a denote the length of the well (8nm). Then the potentia of the particlel is given by

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

Solving the Schodinger Equation for this potential (by separation of variables) yields (see [1]),

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})e^{-i\frac{n^2\pi^2\hbar t}{2ma^2}} \quad \forall n \in \mathbb{N}.$$

The above wavefunctions are referred to as stationary states (the set of all linear combinations of these stationary states is the general solution set of the Schrodinger Equation for this potential). The reason they are called this is because the expected values of quantities such as position and momentum will be independent of time.

3 Position

A postulate of Quantum Mechanics is that $|\Psi|^2$ is the probability density function for the position of the particle. Note this pdf if a real valued function

$$|\Psi|^2 = \Psi^*\Psi = \sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})e^{i\frac{n^2\pi^2\hbar t}{2ma^2}}\sqrt{\frac{2}{a}}\sin(\frac{n\pi x}{a})e^{-i\frac{n^2\pi^2\hbar t}{2ma^2}} = \frac{2}{a}\sin^2(\frac{n\pi x}{a}).$$

Note that this pdf is independent of time. For this reason we will denote $|\Psi|^2$ as $|\psi|^2$. Since $|\psi|^2$ is the probability density function for the position of the particle, then the expected value of the position of the particle is given by: [Note: It is customary to denote expected values in angle brackets in Quantum Mechanics]

$$\langle x \rangle = \int_0^a x|\psi|^2\,dx = \frac{2}{a}\int_0^a x\sin^2(\frac{n\pi x}{2})\,dx$$

$$= \frac{2}{a}\int_0^a x\left[\frac{1-\cos(2n\pi x/a)}{2}\right]\,dx = \frac{1}{a}\int_0^a x\,dx - \frac{1}{a}\int_0^a x\cos(2n\pi x/a)\,dx.$$

Note that

$$\frac{1}{a}\int_0^a x\,dx = \frac{1}{a}\left[\frac{x^2}{2}\right]_0^a = \frac{a}{2}.$$

We use integration by parts to solve the second integral. Let $u = x$ and $dv = \cos(2n\pi x/a)$. Then $du = dx$ and $v = \frac{a}{2n\pi}\sin(2n\pi x/a)$. Hence

$$\frac{1}{a}\int_0^a x\cos(2n\pi x/a)\,dx = \frac{1}{a}\left([uv]_0^a - \int_0^a v\,du\right).$$

Note that uv evaluated at 0 and a is 0 since $\sin(0) = 0$ and $\sin(2n\pi) = 0$ due to n being an integer. Now note that

$$\int_0^a v\,du = \frac{a}{2n\pi}\int_0^a \sin(2n\pi x/a)\,dx = \frac{a^2}{(2n\pi)^2}\left[-\cos(2n\pi x/a)\right]_0^a$$

$$= \frac{a^2}{(2n\pi)^2}(1-\cos(2n\pi)).$$

Recall that $\cos(2n\pi) = 1$ since n is an integer. Hence the integral is 0. Therefore

$$\langle x \rangle = \frac{a}{2}.$$

We now calculate the second moment.

$$\langle x^2 \rangle = \int_0^a x^2|\psi|^2\,dx = \frac{2}{a}\int_0^a \sin^2(n\pi x/a)\,dx = \frac{1}{a}\int_0^a x^2\,dx - \frac{1}{a}\int_0^a x^2\cos(2n\pi x/a)\,dx.$$

Note that

$$\frac{1}{a}\int_0^a x^2\,dx = \frac{1}{a}\frac{a^3}{3} = \frac{a^2}{3}$$

We use integration by parts twice to solve the second integral. Let $u = x^2$ and $dv = \cos(2n\pi x/a)$. Then $du = 2xdx$ and $v = \frac{a}{2n\pi}\sin(2n\pi x/a)$. So

$$\int_0^a x^2\cos(2n\pi x/a)\,dx = \left[x^2\frac{a}{2n\pi}\sin(2n\pi x/a)\right]_0^a - \frac{a}{n\pi}\int_0^a x\sin(2n\pi x/a)\,dx.$$

The uv term evaluates to 0 as before. We now integrate the second integral by parts.

$$\int_0^a x\sin(2n\pi x/a)\,dx = \left[-\frac{xa}{2n\pi}\cos(2n\pi x/a)\right]_0^a + \frac{a}{2n\pi}\int_0^a \cos(2n\pi x/a)\,dx$$

$$= -\frac{a^2}{2n\pi}\cos(2n\pi) = -\frac{a^2}{2n\pi}$$

Hence

$$\frac{1}{a}\int_0^a x^2\cos(2n\pi x/a)\,dx = \frac{1}{a}(\frac{-a}{n\pi})(-\frac{a^2}{2n\pi}) = \frac{a^2}{2(n\pi)^2}$$

So

$$\langle x^2\rangle = \frac{a^2}{3} - \frac{a^2}{2(n\pi)^2} = a^2\left(\frac{1}{3} - \frac{1}{2(n\pi)^2}\right).$$

We now can calculate that standard deviation of the position. The variance is given by

$$\sigma_x^2 = \langle x^2\rangle - \langle x\rangle^2 = a^2\left(\frac{1}{3} - \frac{1}{2(n\pi)^2}\right) - \frac{a^2}{4} = a^2\left(\frac{1}{12} - \frac{1}{2(n\pi)^2}\right) = \frac{a^2}{4}\left(\frac{1}{3} - \frac{2}{(n\pi)^2}\right).$$

Hence the standard deviation is given by

$$\sigma_x = \frac{a}{2}\sqrt{\frac{1}{3} - \frac{2}{(n\pi)^2}}.$$

The pdf of the first 3 stationary states is given as follows:

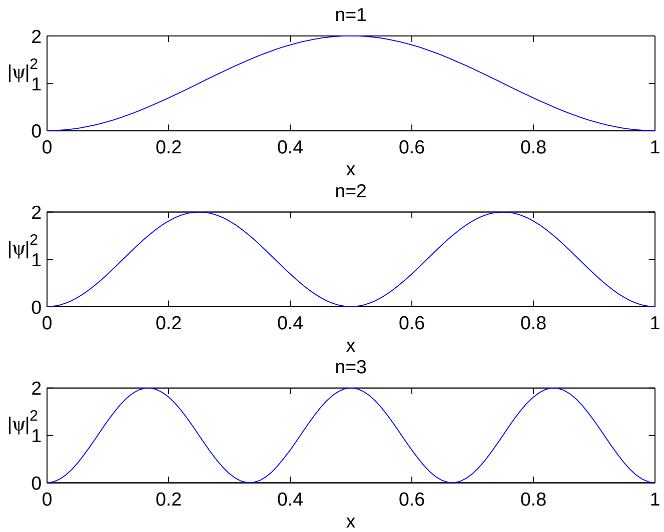

Figure 1: $|\psi|^2$ for $n = 1, 2, 3$

4 Momentum

Recall that classical momentum is given by mass times to time rate of change of position. So since the expected value of position was constant in time, then one may suspect that the the expected value of momentum is 0. It turns out this is that case. It can be proven that

$$\langle p \rangle = m \frac{d}{dx} \langle x \rangle = 0.$$

The exact details of calculating the second moment of momentum will not be dicussed in order to prevent this paper from being too lengthy, but it can be shown (see [1]) that

$$\langle p^2 \rangle = \left(\frac{n\pi\hbar}{a} \right)^2.$$

Hence

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \left(\frac{n\pi\hbar}{a} \right)^2$$

and

$$\sigma_p = \frac{n\pi\hbar}{a}.$$

The probability distribution function of the particles momentum was plotted in MATLAB for the first 3 stationary states (once again details will be excluded regarding the exact functional form of the pdf).

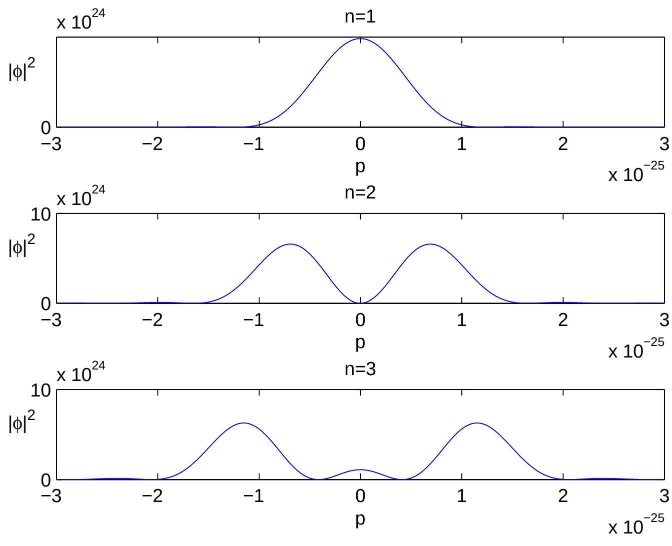

Figure 2: $|\phi|^2$ for $n = 1, 2, 3$

5 Discussion

From the above information we can gather that a particle behaves very different on a quantum mechanical scale compared to one on a classical mechanical scale. In particular, we see that the position of a particle is never known with absolute certainty (unless the particle is observed which will in turn cause the observor to be uncertain of the particles momentum [see Uncertainty Principle below]). From the probability density function of the particle in the infinite square well, we see that the particle is more likely to be in some places than others. For example, a particle is more more likely to be found at the position corresponding to a crest of the pdf rather than a trough. From the expected value of the position we see that if we have numerous identically prepared particles in an infinite potential well, then the average measurement of position will be $\frac{a}{2}$. As we see from our calculation, this expected value is the same for all stationary states. This becomes apparent when we observe the symmetry in the pdf for each state. In addition we see from the standard deviation that for stationary states with a higher n (which actually corresponds to higher energy), the spread of the measurement of position increases (up to $\frac{a}{2}\sqrt{1/3}$). In addition, the spread in momentum increases proportionally with n.

We lastly discuss the uncertainty principle. Note that

$$\sigma_x \sigma_p = \frac{a}{2}\sqrt{\frac{1}{3} - \frac{2}{(n\pi)^2}}\left(\frac{n\pi\hbar}{a}\right) = \frac{\hbar}{2}\sqrt{\frac{(n\pi)^2}{3} - 2}.$$

Heisenberg's Uncertainity Principle states that

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}.$$

Note that $\frac{\hbar}{2} = 5.2728E - 35$. Thus our data from Table 1 agrees with the Uncertainty Principle. Physically we see that if a particle's momentum has a relatively small standard deviation, then the standard deviation of the particles position must be relatively large. This means that gaining certainty in knowing the position of a particle causes there to be a loss of certainity in knowing the momentum of the particle. For example the standard deviation of momentum in our example is around the scale of 10^{-26} kg m/s. However the standard deviation of momentum in our example is around the scale of 10^{-9} m.

n	1	2	3	4	5
σ_x(m)	1.4460E-9	2.1267E-9	2.230E-9	2.2651E-9	2.2811E-9
σ_p (kg m/s)	4.1413E-26	8.2826E-26	1.2424E-25	1.6565E-25	2.0706E-25
$\sigma_x\sigma_p$	5.9885E-35	1.7614E-34	2.7706E-34	3.7522E-34	4.7234E-34

Table 1: Standard Deviations of Position and Momentum

6 References

[1] Griffiths, David J. *Introduction to Quantum Mechanics.* 2nd ed. New Jersey: Pearson, 2005.