PHY140Y

23   Implications of Schrödinger's Wave Functions

23.1   Overview

- Probability Calculations for Particle in a 1D Box

- Energy

- Heisenberg Uncertainty Principle

23.2   Probability Calculations for Particle in a 1D Box

We have found that the possible solutions to Schrödinger's equation for a single particle in a box have the form

$$\psi_n(x) \;\; = \;\; \sqrt{\frac{2}{L}}\,\sin\left(n\pi x/L\right), \tag{1}$$

where $n = 1, 2, 3, \ldots$. In order to see how we can use this expression, let's first look at the probability densities associated with a few of the possible wave functions. We will denote n as the principal quantum number. These are illustrated in Fig. 1. We see that the solutions predict that there are particular parts of the box that it is less likely to find the particle. On the other hand, as n increases, we see that the probability becomes increasingly uniform across the box. This is consistent with what we would have expected in the classical limit.
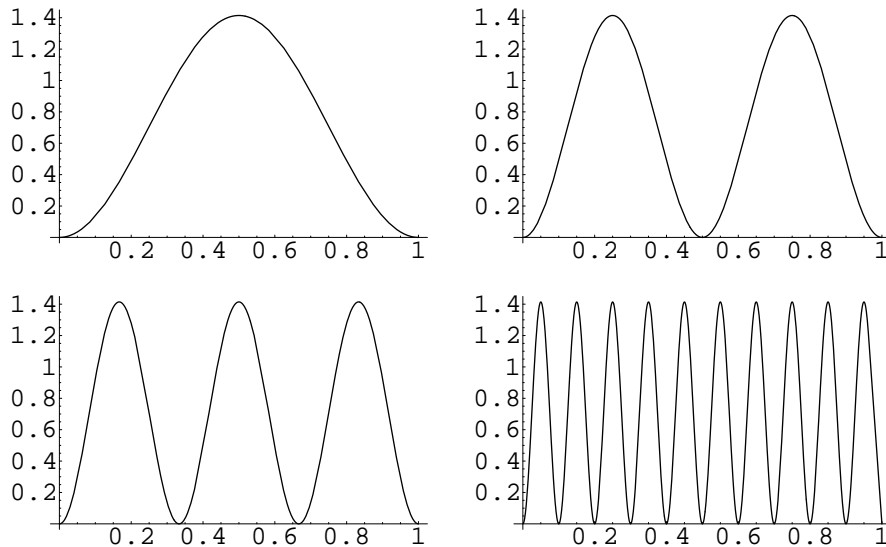

Figure 1: The probability densities for the $n = 1, 2, 3$ and 10 wave functions for the particle in a 1D box.

n	$P_{edge,n}$
1	0.182
2	0.500
3	0.610
4	0.500
11	0.470

Table 1: The probability of finding the particle nearer the edge as a function of the principal quantum number n.

As a concrete, quantitative example, let's calculate how often one would expect to find the particle closer to an edge than the middle.

The condition we are considering is how likely we would find the particle with $x \in (0, L/4)$ or $x \in (3L/4, L)$. Since the probability density is $P(x) = |\psi(x)|^2$, the probability of finding the particle in one of these two intervals when the system is in the nth wave function $\psi_n(x)$ is

$$
\begin{aligned}
P_{edge,n} &= \int_0^{L/4} |\psi_n(x)|^2 dx + \int_{3L/4}^L |\psi_n(x)|^2 dx & (2) \\
&= 2 \int_0^{L/4} |\psi_n(x)|^2 dx & (3) \\
&= 2 \int_0^{L/4} \left(\frac{2}{L}\right) \sin^2 \left(\frac{n\pi x}{L}\right) dx & (4) \\
&= \left(\frac{4}{L}\right) \int_0^{n\pi/4} \left(\sin^2 \eta\right) \left(\frac{L}{n\pi}\right) d\eta & (5) \\
&= \left(\frac{4}{n\pi}\right) \left[\frac{\eta}{2} - \frac{\sin 2\eta}{2}\right]_0^{n\pi/4} & (6) \\
&= \frac{1}{2} - \left(\frac{2}{n\pi}\right) \sin\left(n\pi/2\right), & (7)
\end{aligned}
$$

where we have made a change of variable $\eta \equiv n\pi x/L$. The classical result would have been exactly one-half. In fact, the QM result varies with whatever wave function the system is in. Thus, if we calculate this for various values of n, we get the probabilities listed in Tab. 1. We see that this probability fluctuates depending on what quantum state the system is in.

23.3 Energy

The energy in the 1D box is given by the condition

$$
\begin{aligned}
k_n &= \frac{n\pi}{L} & (8) \\
&= \frac{\sqrt{2mE_n}}{\hbar} & (9) \\
\Rightarrow E_n &= \frac{n^2\pi^2\hbar^2}{2mL^2}, & (10)
\end{aligned}
$$

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so the energy of the system rises like n^2. As a concrete example, suppose that we had an electron in a box had a width of $L = 5.1 \times 10^{-11}$ m (the Bohr radius). Then the lowest possible energy of the electron would be

$$E_1 \;=\; \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) = 2.4 \times 10^{-17} \text{ J} = 150 \text{ eV}. \tag{11}$$

This is a sizeable energy, especially when we consider that the electron in a hydrogen atom is bound with about 10% of is ground state energy.

23.4 Heisenberg Uncertainty Principle

From this expression for the energy, we can also determine the magnitude of the momentum of the particle. It would be given by

$$p_n \;=\; \sqrt{2mE_n} \tag{12}$$
$$\;=\; \frac{\pi \hbar}{L}\, n. \tag{13}$$

Now, we don't know the direction of the particle, so we can estimate the uncertainty in the momentum to be of order twice the momentum itself, or

$$\Delta p \;=\; \frac{2\pi \hbar}{L}\, n. \tag{14}$$

Since the uncertainty in the particle's position is given by the length of the box itself, so that $\Delta x = L$, we find that

$$\Delta x \Delta p \;=\; 2\pi \hbar n \tag{15}$$
$$\Rightarrow \Delta x \Delta p \;\geq\; \hbar. \tag{16}$$

This is an example of the Heisenberg Uncertainty Principle: you can never measure two "conjugate" variables to arbitrary precision. This is Quantum Mechanics way of saying that you are limited in what you can know if you want to measure both position and momentum.

This principle extends to other pairs of "conjugate" variables. Perhaps the most notable are

$$(\theta, \vec{L}) \tag{17}$$
$$(\text{Energy}, \text{time}) \tag{18}$$
$$(x, p) \tag{19}$$

There were a number of thought experiments that illustrated why in practice this principle should rule, but the real issue is that QM will always ensure that you do not violate the Heisenberg Uncertainty principle.