

restart

First, let's define the wavefunction:

$$\psi := (n, x) \rightarrow A \cdot \sin\left(\frac{n \cdot \pi \cdot x}{a}\right)$$

$$(n, x) \rightarrow A \sin\left(\frac{n \pi x}{a}\right) \quad (1)$$

Normalize it!

$$\int_0^a \psi(n, x)^2 dx$$

$$\frac{1}{2} a A^2 \quad (2)$$

Solve for A:

solve(%=1, A)

$$\frac{\sqrt{2}}{\sqrt{a}}, -\frac{\sqrt{2}}{\sqrt{a}} \quad (3)$$

We'll choose the positive root, but either coefficient is possible, since the probability will only depend on the square of this value.

$$A := \sqrt{\frac{2}{a}}$$

$$\sqrt{2} \sqrt{\frac{1}{a}} \quad (4)$$

Let's admire our normalized wavefunction!

$\psi(n, x)$

$$\sqrt{2} \sqrt{\frac{1}{a}} \sin\left(\frac{n \pi x}{a}\right) \quad (5)$$

Let's also double check the normalization:

$$\int_0^a \psi(n, x)^2 dx$$

$$\frac{-\cos(n \pi) \sin(n \pi) + n \pi}{n \pi} \quad (6)$$

Since n is an integer, the first term always vanishes -- $\sin(n \pi) = 0$. Thus, this is indeed normalized.

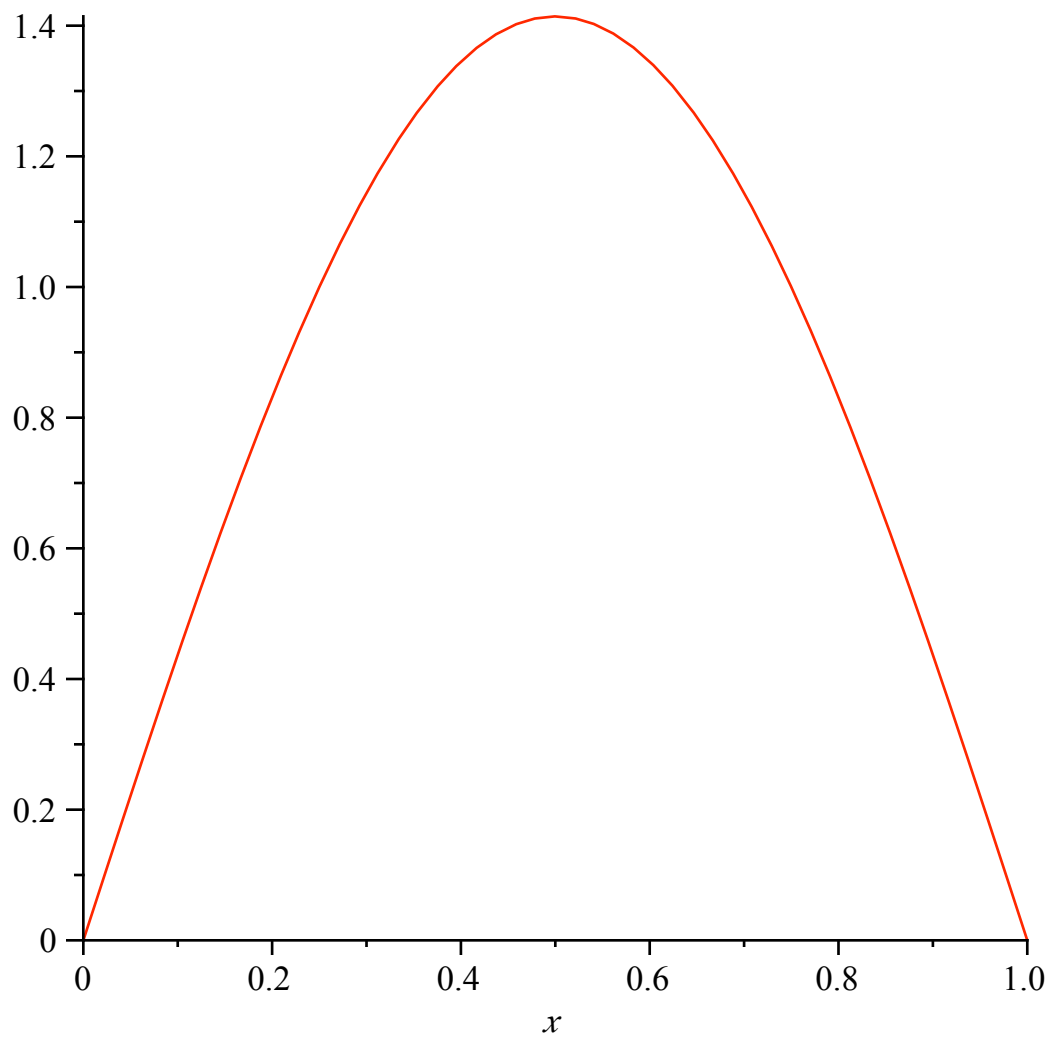
Let's work with some plots. In order to visualize the solutions, we'll need to specify a numerical value for the box size:

$a := 1$

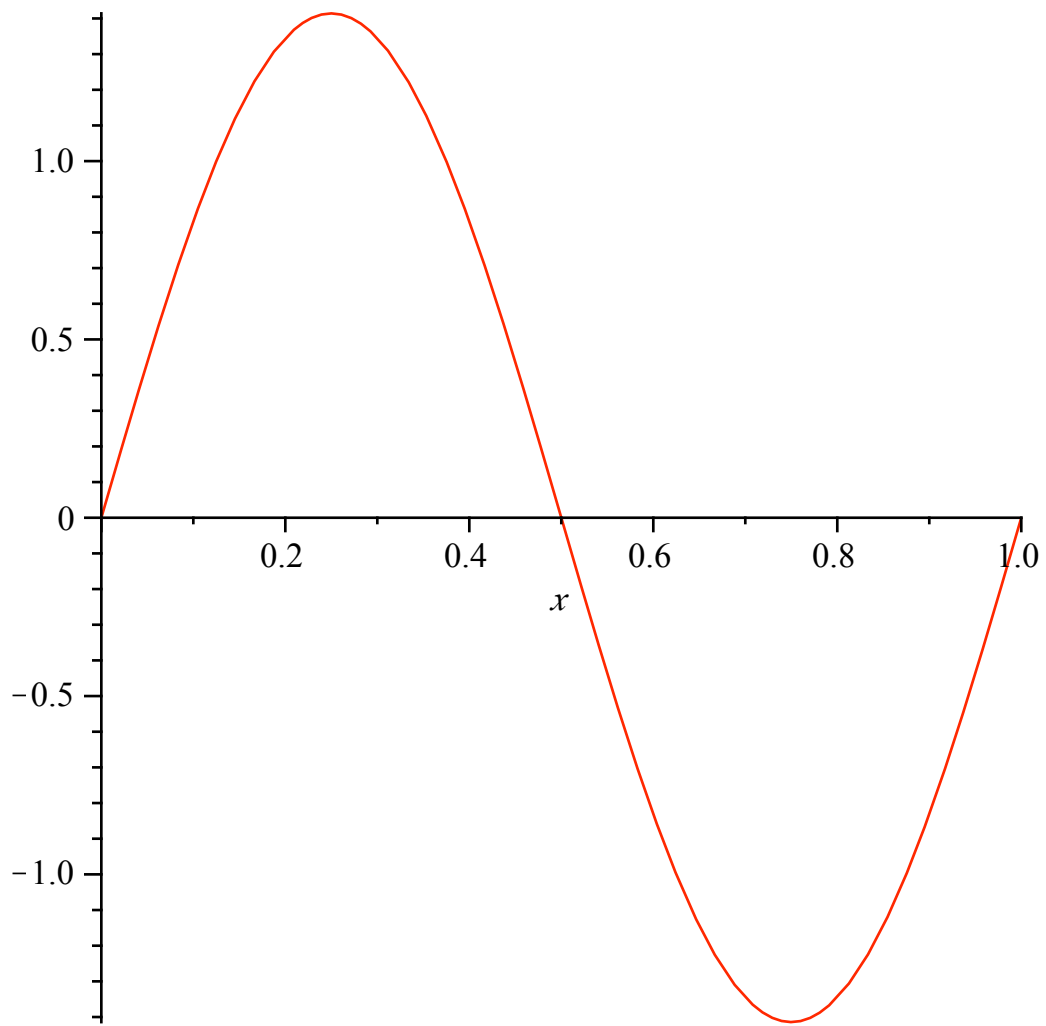
$$1 \quad (7)$$

We can now plot the wavefunctions for arbitrary n :

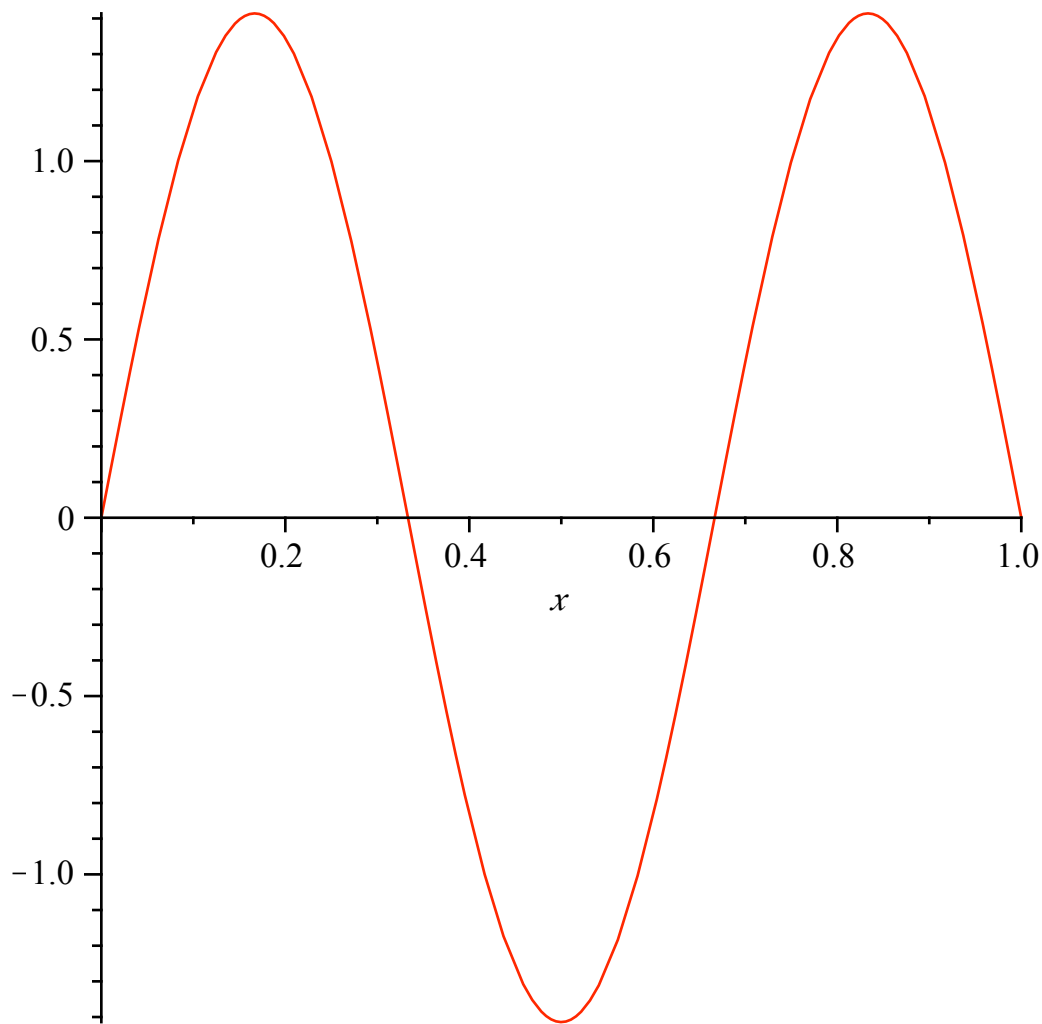
$plot(\psi(1, x), x=0..a)$



plot(psi(2, x), x=0 ..a)



plot(psi(3, x), x=0..1)



Good stuff! We can now calculate probabilities. To evaluate the probability that the particle is between $x=0.5$ and $x=1$, we simply evaluate:

$$\text{int}(\text{psi}(1, x)^2, x=0.5..1) \quad 0.5000000000 \quad (8)$$

$$\text{int}(\text{psi}(2, x)^2, x=0.5..1) \quad 0.5000000000 \quad (9)$$

$$\text{int}(\text{psi}(3, x)^2, x=0.5..1) \quad 0.5000000000 \quad (10)$$

As we expect from the distribution (it's symmetric about $x=0.5$), there is a 50% chance the particle is in this range.

Now let's evaluate the expectation values. Where is the particle most likely to be?

$$X_{\text{expect}} := \int_0^1 x \cdot \text{psi}(1, x)^2 dx \quad \frac{1}{2} \quad (11)$$

In the middle! Of course, we should naturally expect this as well from looking at the distribution.

You can check that the same response is obtained for $n=2, 3$, or any old value.

To calculate the uncertainty in position, we'll also need the expectation value of the *square* of the position operator:

$$X2xpctI := \int_0^a x^2 \cdot \text{psi}(1, x)^2 dx$$

$$\frac{1}{6} \frac{-3 + 2 \pi^2}{\pi^2} \quad (12)$$

By our formula, the uncertainty is thus

$$\Delta X := \sqrt{X2xpctI - XpctI^2}$$

$$\frac{1}{6} \sqrt{\frac{6(-3 + 2 \pi^2)}{\pi^2} - 9} \quad (13)$$

Looks messy, but we can simplify it:

$$\text{evalf}(\%)$$

$$0.1807560274 \quad (14)$$

To evaluate the Heisenberg Uncertainty Principle, we need to know the uncertainty in the momentum as well. So, we proceed as before by evaluating the expectation value of the momentum operator. In this case:

assume($\hbar > 0$)

$$PxpctI := \frac{\hbar}{I} \cdot \int_0^a \text{psi}(1, x) \frac{d}{dx} \text{psi}(1, x) dx$$

$$0 \quad (15)$$

It's zero! Why is that? These solutions are what are known as *stationary states*, so this can be considered a characteristic property. We'll discuss this a bit more later. On to $\langle P^2 \rangle$:

$$P2xpctI := -\hbar^2 \cdot \int_0^1 \text{psi}(1, x) \cdot \frac{d}{dx} \frac{d}{dx} \text{psi}(1, x) dx$$

$$\hbar^2 \pi^2 \quad (16)$$

And finally, the uncertainty:

$$\Delta P := \sqrt{P2xpctI - PxpctI^2}$$

$$\hbar \pi \quad (17)$$

The Heisenberg Uncertainty Principle says....

$$\Delta X \cdot \Delta P$$

$$\frac{1}{6} \sqrt{\frac{6(-3 + 2 \pi^2)}{\pi^2} - 9} \hbar \pi \quad (18)$$

evalf(%)

$$0.5678618078 \hbar \sim$$

(19)

Hurray! It is indeed $\geq \hbar/2$, as we should expect.