In[10]:= `DateList[]`

Out[10]= {2009, 10, 19, 12, 35, 3.457034}

■ Box 0 < x < L -> 2 L

Consider the case when we have a particle in the ground state of PIB of length L.

In[3]:= $$\Psi 1[x\_, L\_] := \sqrt{\frac{2}{L}}\ \mathrm{Sin}\left[\frac{\pi x}{L}\right]$$

Definitions:

In[4]:= $$\Phi[x\_, L\_] := \mathrm{If}[0 < x < L,\ \Psi 1[x, L],\ 0]$$

In[5]:= $$\phi[m\_][x\_, L\_] := \sqrt{\frac{1}{L}}\ \mathrm{Sin}\left[\frac{m \pi x}{2 L}\right]$$

Now we have two normalized functions

In[6]:= $$\int_0^L \Psi 1[x, L]\ \Psi 1[x, L]\ dx$$

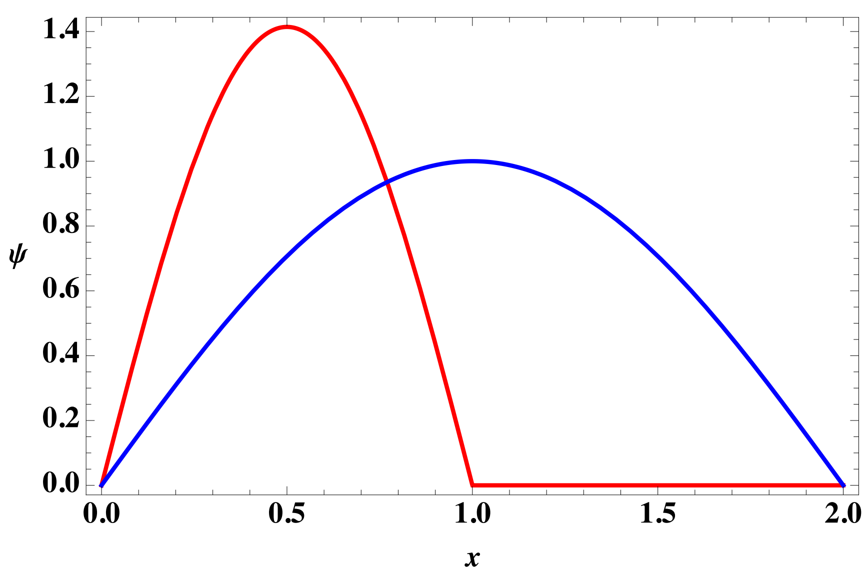
Out[6]= $$1$$

In[7]:= $$\int_0^{2 L} \phi[m][x, L]\ \phi[m][x, L]\ dx$$

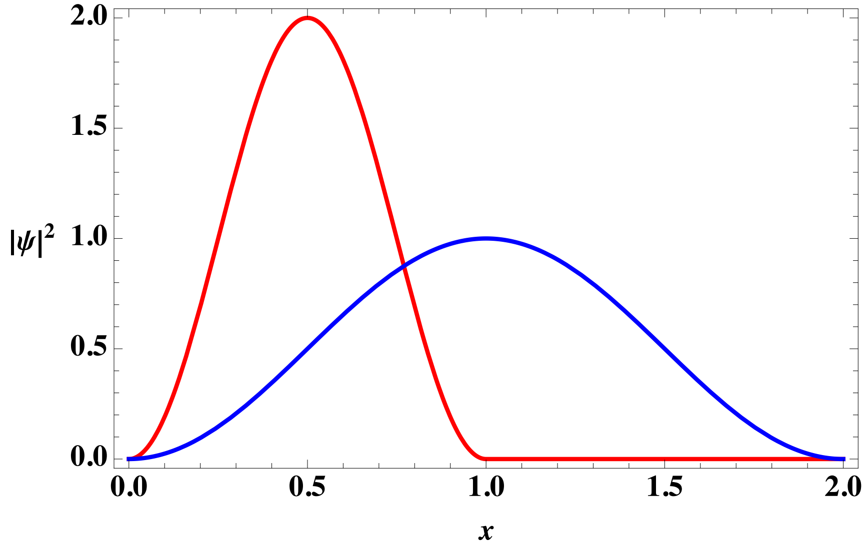
Out[7]= $$1 - \frac{\mathrm{Sin}[2 m \pi]}{2 m \pi}$$

For completeness we plot the functions and the square of the functions, assuming that L =1 .

```
Plot[{Φ[x, 1], (ϕ[1][x, 1])}, {x, 0, 2}, PlotStyle → {{Thick, Red}, {Thick, Blue}},
 BaseStyle → {Bold, 14}, Frame → True, FrameLabel → {x, ψ}, RotateLabel → False, ImageSize → 400]
```



```
Plot[{Ψ[x, 1]^2, (ϕ[1][x, 1]^2)}, {x, 0, 2},
 PlotStyle → {{Thick, Red}, {Thick, Blue}}, BaseStyle → {Bold, 14},
 Frame → True, FrameLabel → {x, "|ψ|²"}, RotateLabel → False, ImageSize → 400]
```



To find the expansion coefficients and the probabilities, we first need to define the coefficients in the new basis set of the bigger box:

In[8]:=

```
c[m_, L_] := Simplify[∫_0^L ϕ[m][x, L] Ψ1[x, L] ⅆx, Assumptions → {m ∈ Integers}]
```

In general the coefficients are given by the following expression:

In[9]:=

```
c[m, L]
```

Out[9]=

$$\frac{4\sqrt{2}\,\mathrm{Sin}\left[\frac{m\pi}{2}\right]}{4\pi - m^2\pi}$$

Notice that n=2 may give us a problem.

Now we calculate the probabilities as the square of the coefficients

```
prob1 = Table[{n, c[n, 1]^2} // N, {n, 1, 10}];
```

and show them in a tabular form

```
TableForm[prob1, TableHeadings →
  {{"n =", "n =", "n =", "n =", "n =", "n =", "n =", "n =", "n =", "n ="}, {n, Prob1}}]
```

	n	Prob1
n =	1.	0.360253
n =	2.	0.5
n =	3.	0.129691
n =	4.	0.
n =	5.	0.0073521
n =	6.	0.
n =	7.	0.00160112
n =	8.	0.
n =	9.	0.000546851
n =	10.	0.

From the table we notice that the probability of finding the particel in the grouns state of the bigger box is only 36% compared to 50% in the first exicted state. Furthermore we can calculate the sum of the square of the coefficients and include up to 50 terms

$$\textbf{probT1} = \sum_{m=1}^{50} c[m, L]^2 // N$$

0.999996

We can also calcuate the average energy

$$\textbf{averE} = N\left[\sum_{m=1}^{50} c[m, L]^2\, m^2 / 4\right]$$

0.991887

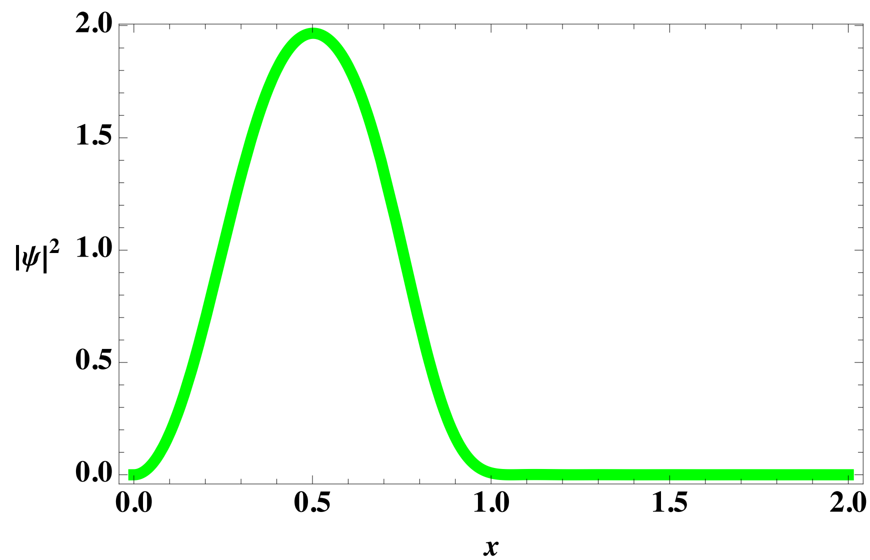
Finally we construct the approximate wave function thet include the contribution of the first 10 eigenfunctions of the bogger box

$$\textbf{aproxF}[x\_, L\_] = \sum_{m=1}^{10} c[m, L]\, \phi[m][x, L]$$

$$\frac{4\sqrt{2}\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{\pi x}{2L}\right]}{3\pi} + \frac{\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{\pi x}{L}\right]}{\sqrt{2}} + \frac{4\sqrt{2}\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{3\pi x}{2L}\right]}{5\pi} - \frac{4\sqrt{2}\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{5\pi x}{2L}\right]}{21\pi} + \frac{4\sqrt{2}\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{7\pi x}{2L}\right]}{45\pi} - \frac{4\sqrt{2}\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{9\pi x}{2L}\right]}{77\pi}$$

Let us plot the approximate wave function

```
Plot[aproxF[x, 1]^2, {x, 0, 2}, PlotStyle → {Green, Thickness[0.015]}, BaseStyle → {Bold, 14},
 Frame → True, FrameLabel → {x, "|ψ|^2"}, RotateLabel → False, ImageSize → 400]
```



If we measure the energy in units of ue

$$ue = \frac{h^2}{8\,m\,L^2}$$

and time in units of

$$ut = \frac{8\,m\,L^2}{h}$$

we can construct the approximate time dependent wave function

$$\text{aprox}[x\_, 1, t\_] = \sum_{m=1}^{10} c[m, 1]\,\phi[m][x, 1]\,\text{Exp}[-i\,m^2\;2\,\pi\,t/4]$$

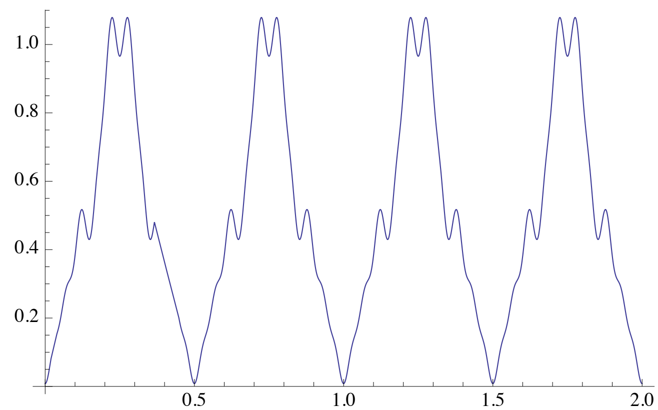
$$\frac{4\sqrt{2}\,e^{-\frac{1}{2} i \pi t}\,\text{Sin}\left[\frac{\pi x}{2}\right]}{3\pi} + \frac{e^{-2 i \pi t}\,\text{Sin}[\pi x]}{\sqrt{2}} + \frac{4\sqrt{2}\,e^{-\frac{9}{2} i \pi t}\,\text{Sin}\left[\frac{3\pi x}{2}\right]}{5\pi} - \frac{4\sqrt{2}\,e^{-\frac{25}{2} i \pi t}\,\text{Sin}\left[\frac{5\pi x}{2}\right]}{21\pi} + \frac{4\sqrt{2}\,e^{-\frac{49}{2} i \pi t}\,\text{Sin}\left[\frac{7\pi x}{2}\right]}{45\pi} - \frac{4\sqrt{2}\,e^{-\frac{81}{2} i \pi t}\,\text{Sin}\left[\frac{9\pi x}{2}\right]}{77\pi}$$

But we really want to visualize the probabilitydensity of finding the particel at x

```
prob[x_, 1, t_] = Simplify[Expand[aprox[x, 1, t] * aprox[x, 1, -t]]]
```

Now we consider the middle of the box and consider the probability as a function of time

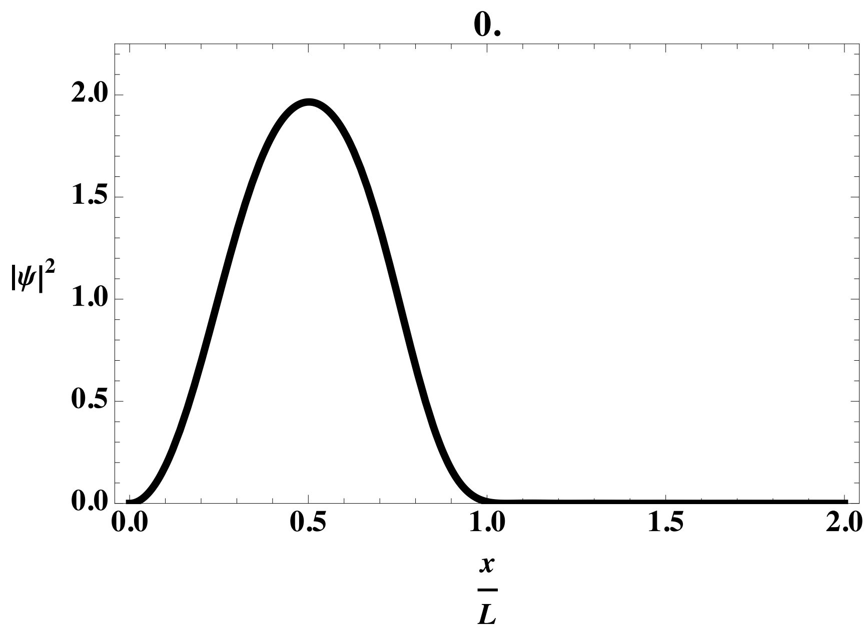
```
Plot[Evaluate[Re[prob[1, 1, t]]], {t, 0, 2}]
```



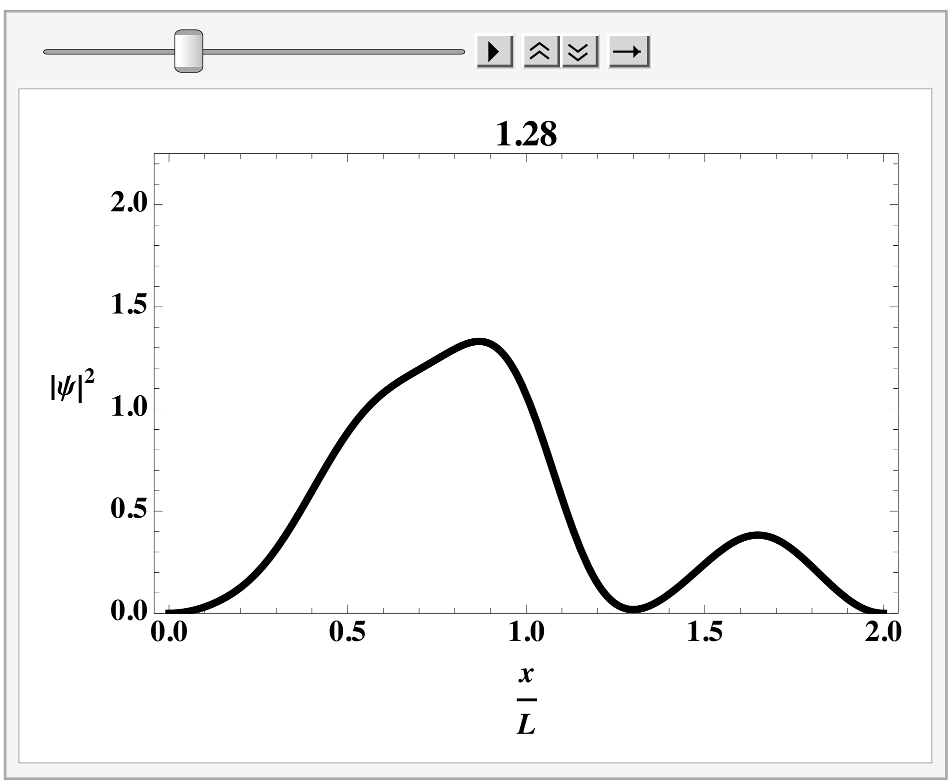

```
movie = Table[Plot[Evaluate[Re[prob[x, 1, n]]], {x, 0, 2},
    PlotRange -> {0, 2.25}, Frame → True, ImageSize → 400, PlotLabel → N[n],
    FrameLabel → {x / L, "|ψ|²"}, PlotPoints → 100, RotateLabel → False,
    PlotStyle → {Black, Thickness[0.01]}, BaseStyle → {Bold, 14}], {n, 0, 4, 1 / 100}];
```

Movie: Using printed plots from movie, selecting the cell and saving selection from **File->Save Selection As** menu as QuickMovie, or select all the figures and use **Cell -> ConverTo.-> QuickTime.** Also we can animate the cell using **Graphics->Rendering->Animate**, but **ListManipulate** is better

```
Do[Print[movie[[i]]], {i, 1, Length[movie]}](*Flush the figures to the left*)
```




```
ListAnimate[movie]
```



- **Box -L/2 < x < L/2 -> -L < x < L**

PARTICLE IN A BOX REVISITED

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}[V - E]\psi$$

$$s = \frac{x}{L} \qquad x = L\,s$$

$$0 < s < 1 \qquad dx = L\,ds$$

$$\frac{1}{L^2}\frac{d^2\psi}{ds^2} = \frac{8m\,\pi^2}{h^2}[V - E]\psi$$

$$\frac{d^2\psi}{ds^2} = \pi^2[\upsilon - \varepsilon]\psi = k^2\psi$$

$$u_e = \frac{h^2}{8mL^2} \Rightarrow \varepsilon = \frac{E}{u_e}$$

$$\upsilon = \frac{V}{u_e}$$

$$\boxed{k = \pi\sqrt{\upsilon - \varepsilon}}$$

$$k = \pi\sqrt{\varepsilon} \qquad V = 0$$

$$\boxed{\Psi_n(s) = \sqrt{2}\,\sin(n\pi s)} \qquad \varepsilon = n^2$$

$$uE \simeq \frac{h^2}{8mL^2}$$

$$ut = \frac{8mL^2}{h}$$

FOR $m = m_e$

$L = 500\ pm$

$L = 5 \times 10^{-10}\ m$

$$uE \sim 1.5\ eV$$

$$ut \sim 2.7\ ft = 2.7 \times 10^{-15}\ s$$

Consider

$$\hat{H}\phi_n = E_n\phi_n$$

SINCE $\hat{H}$ IS THE HAMILTONIAN WITH REAL EIGENVALUES, ϕ_n ARE ORTHOGONAL, SO IF WE NORMALIZE THEM, WE GET A COMPLETE SET $\{\Phi_n\}$, WHERE

$$\langle\Phi_n|\Phi_m\rangle \equiv \langle n|m\rangle = \delta_{n,m}$$

FOR THE GENERAL CASE OF A WAVE FUNCTION $\Psi(x)$ WE CAN FIND

$$\Psi(x) = \sum_m C_m \Phi_m$$

with

$$C_m = \int_V \Phi_n^*(x)\,\Psi(x)\,dx \equiv \langle n|\Psi\rangle$$

$$\Psi(x) \equiv \langle x|\Psi\rangle = \sum_m C_m \phi_m(x) = \sum_m \langle m|\Psi\rangle\langle x|m\rangle$$

OR

$$|\Psi\rangle = \sum_m \langle m|\Psi\rangle\,|m\rangle$$

The time dependent wave function $\Psi(x,t)$ is GIVEN by

$$\Psi(x,t) = \sum_m C_m\, e^{-\frac{E_m}{\hbar}t}\,\phi_m(x)$$

NOTICE THAT

$$\hat{H}\Psi(x,t) = \sum_m C_m e^{-\frac{iE_m t}{\hbar}} \hat{H}\phi_n(x)$$

$$= \sum_m E_m C_m e^{-\frac{iE_m t}{\hbar}} \phi_m(x)$$

AND

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \sum_m E_m C_m e^{-\frac{iE_m t}{\hbar}} \phi_m(x)$$

OR

$$\hat{H}\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}.$$