A “Smooth” Piecewise Function

The wave function $\Psi(x)$

We start by defining our piecewise function,

In[1]:=
```
$Assumptions = {n > 0, L > 0, ℏ > 0, Element[{A, L, k, ℏ}, Reals]}
```
Out[1]=
```
{n > 0, L > 0, ℏ > 0, (A | L | k | ℏ) ∈ Reals}
```

In[2]:=
```
Ψu = Piecewise[{{A (x^2 - L^2)^2, x > -L && x < L}}]
```
Out[2]=

$$\begin{cases} A\left(-L^2+x^2\right)^2 & x > -L \,\&\&\, x < L \\ 0 & \text{True} \end{cases}$$

and normalizing it. Notice that this function and its first derivative are continuous.

In[3]:=
```
Anorm = FullSimplify[Solve[Integrate[Abs[Ψu]^2 , { x, -Infinity, Infinity}] == 1, A]]
Ψ = Ψu /. Anorm[[2]][[1]];
```
Out[3]=

$$\left\{\left\{A \to -\frac{3\sqrt{35}}{16\, L^{9/2}}\right\}, \left\{A \to \frac{3\sqrt{35}}{16\, L^{9/2}}\right\}\right\}$$

which is a mess, so we’ll keep using Ψ_u.
With that done, we can take the Fourier transform to find $\tilde{\Psi}$.

In[5]:=
```
Ψ̃u = 1 / Sqrt[2 π] FullSimplify[Integrate[Ψu Exp[-I k x], { x, -Infinity, Infinity}]]
Ψ̃ = Ψ̃u /. Anorm[[2]][[1]];
```
Out[5]=

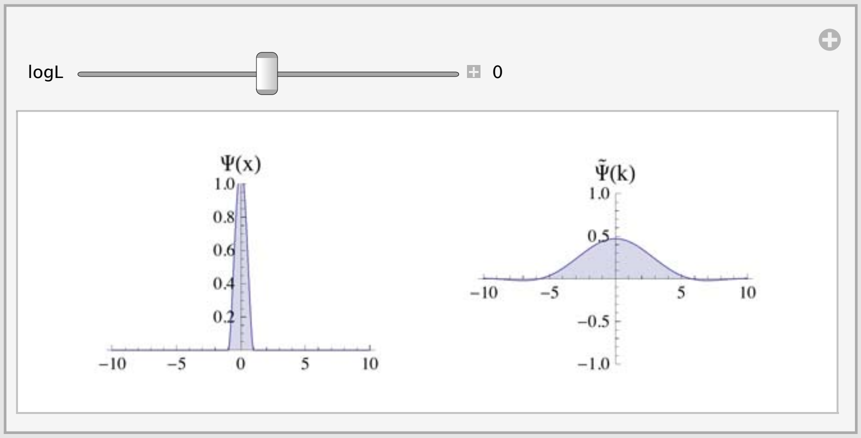
$$-\frac{8\, A \sqrt{\frac{2}{\pi}} \left(3\, k\, L \operatorname{Cos}[k\, L] + \left(-3+k^2 L^2\right) \operatorname{Sin}[k\, L]\right)}{k^5}$$

And to get a feel for this, let’s plot Ψ along with $\tilde{\Psi}$. Both of them are real, so no complications.

In[7]:=

```
Manipulate[
 GraphicsRow[{Plot[Ψ /. {L → 10^logL}, {x, -10, 10}, PlotRange → {0, 1}, Filling → Axis,
     ImageSize → Small, PerformanceGoal → Quality, PlotLabel → "Ψ(x)"],
   Plot[Ψ̃ /. {L → 10^logL}, {k, -10, 10}, PlotRange → {-1, 1},
     Filling → Axis, PerformanceGoal → Quality, PlotLabel → "Ψ̃(k)"]}],
 {{logL, 0}, -1, 1, 0.1, Appearance → "Labeled"}]
```

Out[7]=



Wave function statistics

The usual probability distributions...

In[8]:=

```
FullSimplify[{Px = Abs[Ψ]^2, Pk = Abs[Ψ̃]^2}]
```

Out[8]=

$$\left\{\begin{cases} \frac{315\,(L^2-x^2)^4}{256\,L^9} & L+x>0\ \&\&\ L>x \\ 0 & \text{True} \end{cases},\ \frac{315\,\mathrm{Abs}\left[\frac{3\,k\,L\,\mathrm{Cos}[k\,L]+(-3+k^2\,L^2)\,\mathrm{Sin}[k\,L]}{k^5}\right]^2}{2\,L^9\,\pi}\right\}$$

Let's compute some statistics on this wave function. It is clear from symmetry that <x> = 0 and <k> = 0, but let's write the integrals anyway.

In[9]:=

```
x̄ = Integrate[x Px, {x, -Infinity, Infinity}]
k̄ = Integrate[k Pk, {k, -Infinity, Infinity}]
```

Out[9]= 0

Out[10]= 0

It is less clear what the uncertainties are in x and k. Let's start with Δx...

In[11]:=
```
Δx = Simplify[Sqrt[Integrate[(x - x̄)^2 Px, {x, -Infinity, Infinity}]]]
```
Out[11]=
$$\frac{L}{\sqrt{11}}$$

Great. Onto Δk...

In[12]:=
```
Δk = Simplify[Sqrt[Integrate[(k - k̄)^2 Pk, {k, -Infinity, Infinity}]]]
```
Out[12]=
$$\frac{\sqrt{3}}{L}$$

We find Δx Δk > 1/2, but not by much!

In[13]:=
```
{Simplify[Δx Δk], N[Simplify[Δx Δk]]}
```
Out[13]=
$$\left\{\sqrt{\frac{3}{11}}, 0.522233\right\}$$

The momentum operator $\hat{p}$

Let's try out this new trick, the momentum operator $\hat{p} = -i\,\hbar\,\partial_x$.

In[14]:=
```
pPsi = -I ℏ ∂x Ψ   (* derivative is continuous *)
```
Out[14]=
$$-i\,\hbar\left(\begin{cases}\frac{3\sqrt{35}\,x\,(-L^2+x^2)}{4\,L^{9/2}} & L+x>0\,\&\&\,L-x>0\\ 0 & \text{True}\end{cases}\right)$$

In[15]:=
```
p̄ = Integrate[Ψ* (-I ℏ ∂x Ψ), {x, -Infinity, Infinity}]
```
Out[15]=
0

In[16]:=
```
p2Psi = -ℏ^2 ∂x ∂x Ψ  (* second derivative is NOT continuous at x = ±L *)
```
Out[16]=
$$-\hbar^2\left(\begin{cases}\frac{3\sqrt{35}\,x^2}{2\,L^{9/2}}+\frac{3\sqrt{35}\,(-L^2+x^2)}{4\,L^{9/2}} & L+x>0\,\&\&\,L-x>0\\ 0 & \text{True}\end{cases}\right)$$

In[17]:=
```
p2̄ = Integrate[Ψ* (-I ℏ ∂x (-I ℏ ∂x Ψ)), {x, -Infinity, Infinity}]
```
Out[17]=
$$\frac{3\,\hbar^2}{L^2}$$

In[18]:=

```
Δp = Simplify[Sqrt[p2 - p^2]]
```

$$\Delta p = \text{Simplify}\left[\text{Sqrt}\left[\overline{p2} - \overline{p}^2\right]\right]$$

Out[18]=

$$\frac{\sqrt{3}\,\hbar}{L}$$

Which is what we expect, since $p = \hbar k$.

8.04 Quantum Physics I
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