Wave Functions: A wave-packet

Somehow, in this transition from classical mechanics (CM) to quantum mechanics (QM), we have lost our friends position and momentum (x and p). Here I will show that we haven't really lost them, they are just a little less certain in QM.

The wave function Ψ(x)

We start with a wave function with three parts: an amplitude A, a Gaussian envelope $e^{-\frac{(x-x0)^2}{2d}}$, and a phase oscillation $e^{i\,k0\,(x-x0)}$. The envelope will serve as the position of our particle; we know it is somewhere around x0, with an uncertainty of d. The oscillation with wave number k0 serves as our momentum, since de Broglie tells us that p = $\hbar$k.

In[1]:=

```
Ψu = A Exp[- (x - x0) ^2 / (2 d^2)] Exp[I k0 (x - x0)]
```

Out[1]=

$$A\, e^{i\,k0\,(x-x0)-\frac{(x-x0)^2}{2\,d^2}}$$

(To keep *Mathematica* happy, we need to make explicit some assumptions about our parameters...)

In[2]:=

```
$Assumptions = {d > 0, Element[{x, x0, k0, d}, Reals]}
```

Out[2]=

```
{d > 0, (x | x0 | k0 | d) ∈ Reals}
```

Before we get much further, let's normalize the wave function. By normalizing Ψ(x) we ensure that the probability of finding our particle *somewhere* is equal to 1.

In[3]:=

```
Px = Abs[Ψu]^2;
Anorm = Solve[Integrate[Px, { x, -Infinity, Infinity}] == 1, A]
```

Out[4]=

$$\left\{\left\{A \to -\frac{1}{\sqrt{d}\,\pi^{1/4}}\right\}, \left\{A \to \frac{1}{\sqrt{d}\,\pi^{1/4}}\right\}\right\}$$

We find that there are 2 possible values of A, one positive and one negative. There is no way to say which is correct, since in the end we can only measure $|\Psi(x)|^2$ which means we only care about A^2. Let's update Ψ(x) with the positive value of A.

In[5]:=

```
Ψ = Ψu /. Anorm[[2]]
```

Out[5]=

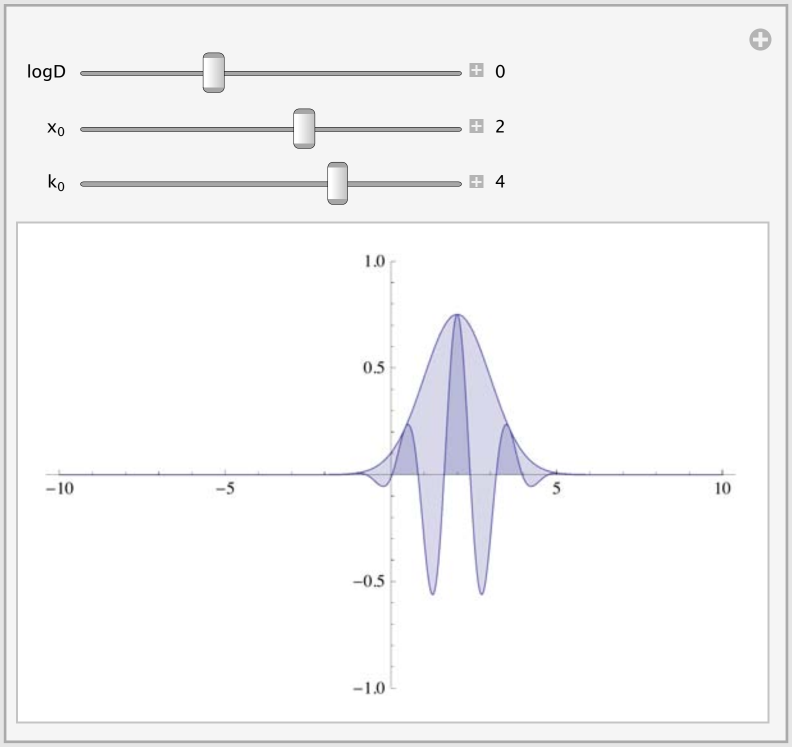
$$\frac{e^{i\,k0\,(x-x0)-\frac{(x-x0)^2}{2\,d^2}}}{\sqrt{d}\,\pi^{1/4}}$$

So that we can see what we are doing, here is a plot of the real part and magnitude of Ψ(x). To move the particle around, change x_0. To make a well-localized particle with low average momentum, make d small (e.g., logD = -1) and k_0 close to 0. Making d large (e.g., logD = 2) moving k_0 away from zero makes a plane-wave-like wave function.

In[6]:=

```
Manipulate[Plot[{Re[Ψ], Abs[Ψ]} /. {A → 1, d → 10^logD, x0 → x₀, k0 → k₀},
   {x, -10, 10}, PlotRange → {-1, 1}, Filling → Axis, PerformanceGoal → Quality],
 {{logD, 0}, -1, 2, 0.1, Appearance → "Labeled"},
 {{x₀, 2}, -10, 10, 0.1, Appearance → "Labeled"},
 {{k₀, 4}, -10, 10, 0.1, Appearance → "Labeled"}]
```

Out[6]=



The Fourier Transform of $\Psi(x)$, $\tilde{\Psi}(k)$

The position-space wave function Ψ(x), shown above, gives us a good idea of the uncertainty in x, but not a lot of information about the uncertainty in p. To get this, let's take the Fourier transform of Ψ(x) to find $\tilde{\Psi}(k)$.

In[7]:=

```
Ψ̃ = 1 / Sqrt[2 π] Integrate[Ψ Exp[-I k x], {x, -Infinity, Infinity}]
```

Out[7]=

$$\frac{\sqrt{d}\ e^{-\frac{1}{2} d^2 (k-k0)^2 - i\,k\,x0}}{\pi^{1/4}}$$

This momentum-space wave function $\tilde{\Psi}(k)$, can be separated in a way similar to $\Psi(x)$... amplitude, envelope, phase.

In[8]:=

$$\tilde{\Psi} == \frac{\sqrt{d}}{\pi^{1/4}} \times e^{-\frac{1}{2} d^2 (k-k0)^2} \times e^{-i\,k\,x0}$$

Out[8]=

```
True
```

And it is properly normalized! (Has anyone heard of Parseval's Theorem?)

In[9]:=

```
Integrate[Abs[Ψ̃]^2, {k, -Infinity, Infinity}]
```

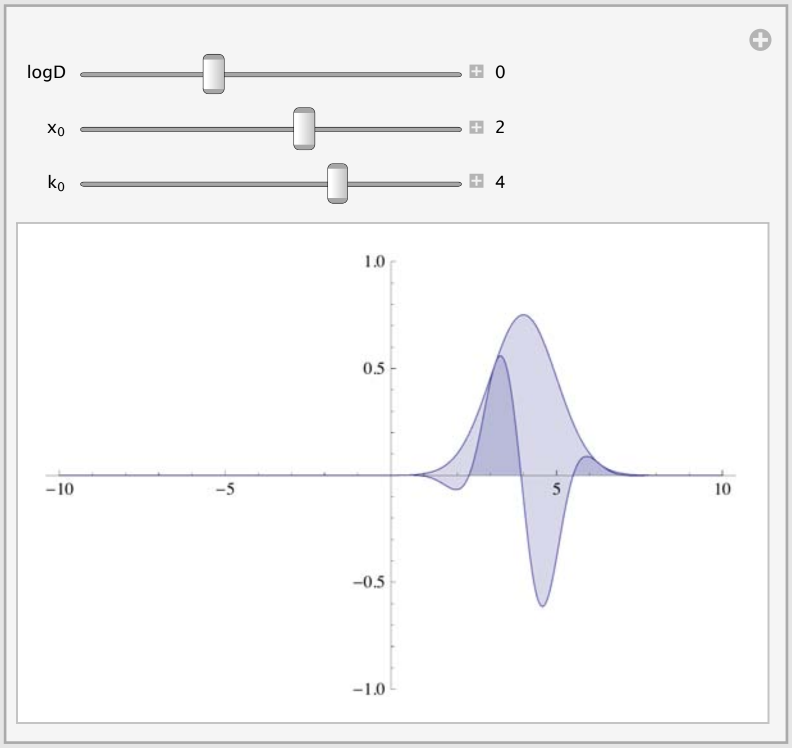
Out[9]=

```
1
```

In[10]:=

```
Manipulate[Plot[{Re[Ψ̃], Abs[Ψ̃]} /. {d → 10^logD, x0 → x₀, k0 → k₀},
   {k, -10, 10}, PlotRange → {-1, 1}, Filling → Axis, PerformanceGoal → Quality],
  {{logD, 0}, -1, 2, 0.1, Appearance → "Labeled"},
  {{x₀, 2}, -10, 10, 0.1, Appearance → "Labeled"},
  {{k₀, 4}, -10, 10, 0.1, Appearance → "Labeled"}]
```

Out[10]=



You can see that the equation for $\tilde{\Psi}(k)$ is essentially identical to Ψ(x) (only an overall phase of $e^{i\,k0\,x0}$ is missing). In particular, the uncertainty in k is now clear; the width of the Gaussian in frequency space is inversely proportional to d, so a narrow peak in Ψ(x) leads to a wide peak in $\tilde{\Psi}(k)$! Putting this all together we see that $\Delta x = d/\sqrt{2}$ and $\Delta k = 1/\sqrt{2}\,d$ such that $\Delta x\,\Delta k = 1/2$, which de Broglie tells us means $\Delta x\,\Delta p = \hbar/2$. **Implication: the Uncertainty Principal need not be an axiom. It is simply the result of the mixed wave-particle nature of reality.**

The Inverse Fourier Transform of $\tilde{\Psi}(k)$

Just to show that it works, let's take the inverse Fourier transform of $\tilde{\Psi}(k)$ to get back to $\Psi(x)$...

In[11]:=

```
Ψ2 = 1 / Sqrt[2 π] Integrate[Ψ̃ Exp[I k x], { k, -Infinity, Infinity}]
```

Out[11]=

$$\frac{e^{\frac{(x-x0)\left(2\,i\,d^2\,k0-x+x0\right)}{2\,d^2}}}{\sqrt{d}\;\pi^{1/4}}$$

In[12]:=

```
Simplify[Ψ2 == Ψ]
```

Out[12]=

```
True
```