Notes for Quantum Mechanics

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Lecture 16

Now remember that before we got $\langle x'|\, \hat{\boldsymbol{p}}\,|\,\alpha\rangle = \frac{\hbar}{i}\frac{d}{dx'}\langle x'|\alpha\rangle$ and I told you we could associate $\langle \mathbf{x'}|\alpha\rangle$ with $\psi(\mathbf{x'})$?

Lets look at this a bit more - remember $\hat{X}|x'\rangle = x'|x'\rangle$ and $\langle x'|x''\rangle = \delta(x'-x'')$. We can write

$|\alpha\rangle = \int dx' \,|\, x'\rangle\langle x'|\alpha\rangle$ and together with the normalization condition $\int dx' \,|\langle x'|\alpha\rangle|^2 = 1$ we can think of $P_\alpha(x')dx' = |\langle x'|\alpha\rangle|^2 dx'$ as being a probability of being between x' and x'+dx so if $|\psi_\alpha(x)|^2$ is thought of as a probability (this is what Bohr said) then $\psi_\alpha(\mathbf{x'}) = \langle \mathbf{x'}|\alpha\rangle$

So now lets consider

$\langle\beta|\alpha\rangle = \int dx' \langle\beta|x'\rangle\langle x'|\alpha\rangle = \int dx'\ \psi_\beta^*(x')\psi_\alpha(x')$. Now the RHS of this thing can be thought of as the overlap in space of the two wave functions - Notice though that the LHS has no x', i.e. it has no space coordinate. We say that it is independent of representation and that it is the probability amplitude that state $|\alpha\rangle$ is to be found in state $|\beta\rangle$ INDEPENDENT OF REPRESENATION. Once we write $\psi_\alpha(\mathbf{x'}) = \langle \mathbf{x'}|\alpha\rangle$ we have chosen the x representation.

So what about operators?. We got a hint from above looking at the x representation of p. Let look at $\langle\beta\,|\,\hat{A}\,|\,\alpha\rangle$

$\langle\beta\,|\,\hat{A}\,|\,\alpha\rangle = \int dx' \int dx'' \langle\beta|x'\rangle \langle x'\,|\,\hat{A}\,|\,x''\rangle\langle x''|\alpha\rangle = \int dx' \int dx''\ \psi_\beta^*(x')\langle x'\,|\,\hat{A}\,|\,x''\rangle\psi_\alpha(x'')$ so what we need is $\langle x'\,|\,\hat{A}\,|\,x''\rangle$ [note that if we wrote this thing in matrix notation - it would be infinite dimensional!]

Now suppose $\hat{A} = \hat{X}^2$ then $\langle x'\,|\,\hat{A}\,|\,x''\rangle = \langle x'\,|\,\hat{X}^2\,|\,x''\rangle = x''^2\delta(x'-x'') = x'^2\delta(x'-x'')$ so

$\langle\beta\,|\,\hat{X}^2\,|\,\alpha\rangle = \int dx' \int dx'' \langle\beta|x'\rangle \langle x'\,|\,\hat{X}^2\,|\,x''\rangle\langle x''|\alpha\rangle = \int dx' \int dx''\ \psi_\beta^*(x')x'^2\delta(x'-x'')\psi_\alpha(x'') = \int dx'\ \psi_\beta^*(x')x'^2\psi_\alpha(x')$

and similarly $\langle\beta\,|\,\hat{X}^n\,|\,\alpha\rangle = \int dx'\ \psi_\beta^*(x')x'^n\psi_\alpha(x')$

Now we can always expand f(x) in a power series so $f(x) = \sum_n a_n x^n$

So $\langle\beta\,|\, f(\hat{X})\,|\,\alpha\rangle = \int dx'\ \psi_\beta^*(x')\ f(x')\psi_\alpha(x')$

Now lets revisit the momentum operator in the position representation (or position basis)

$\langle x'|\,\hat{\boldsymbol{p}}\,|\,\alpha\rangle = \frac{\hbar}{i}\frac{d}{dx'}\langle x'|\alpha\rangle$ so then $\langle x'|\,\hat{\boldsymbol{p}}\,|\,x''\rangle = \frac{\hbar}{i}\frac{d}{dx'}\langle x'|x''\rangle = \frac{\hbar}{i}\frac{d}{dx'}\delta(x'-x'')$

$\langle\beta\,|\,\hat{\boldsymbol{p}}\,|\,\alpha\rangle = \int dx' \int dx'' \langle\beta|x'\rangle \langle x'\,|\,\hat{\boldsymbol{p}}\,|\,x''\rangle\langle x''|\alpha\rangle = \int dx' \int dx''\ \psi_\beta^*(x')\frac{\hbar}{i}\frac{d}{dx'}\delta(x'-x'')\psi_\alpha(x'') = \int dx'\ \psi_\beta^*(x')\frac{\hbar}{i}\frac{d}{dx'}\psi_\alpha(x')$

and we see that in the position representation, the $\hat{\boldsymbol{p}}$ operator just takes the derivative of the wave function in the position representation $\psi_\alpha(x')$

we can also get $\langle x'|\,\hat{\boldsymbol{p}}^n\,|\,\alpha\rangle = \left(\frac{\hbar}{i}\right)^n\left(\frac{d}{dx'}\right)^n\langle x'|\alpha\rangle$ so $\langle\beta\,|\,\hat{\boldsymbol{p}}^n\,|\,\alpha\rangle = \int dx'\ \psi_\beta^*(x')\left(\frac{\hbar}{i}\right)^n\left(\frac{d}{dx'}\right)^n\psi_\alpha(x')$

OK. A natural question to ask is whether we can use some other basis to do all this - how about the momentum basis?

$\hat{P}_{\boldsymbol{i}}|p_i'\rangle = p_i'|p_i'\rangle$ where I have explicitly given the index i=1,2,3 which stands for x,y and z. I will drop this for now.

So we have $\hat{P}|p'\rangle = p'|p'\rangle$ and $\langle p'|p''\rangle = \delta(p'-p'')$. We will expand as usual

$|\alpha\rangle = \int dp' \,|\, p'\rangle\langle p'|\alpha\rangle$ and together with the normalization condition $\int dp' \,|\langle p'|\alpha\rangle|^2 = 1$

so we get $\phi_\alpha(\text{p}') = \langle \text{p}'|\alpha\rangle$ which is now the wave function for $|\alpha\rangle$ in momentum representation.

Is there a way to change basis from position to momentum? Remember to change basis between we need $|b_i\rangle = \hat{U}|a_i\rangle$. By construction we got (lecture 13) $\sum_k |b_k\rangle\langle a_k|$ which if you write this matrix in either basis i.e. $\langle a_j|\hat{U}|a_i\rangle = \langle a_j|b_i\rangle$. So we will need to find $\langle \text{x}'|\text{p}'\rangle$. So let $|\alpha\rangle = |\text{p}'\rangle$ and we get

$\langle \text{x}'|\,\hat{\text{p}}\,|p'\rangle = \frac{\hbar}{i}\frac{d}{\text{dx}'}\langle \text{x}'|\text{p}'\rangle \quad \Longrightarrow \quad \text{p}'\langle \text{x}'|p'\rangle = \frac{\hbar}{i}\frac{d}{\text{dx}'}\langle \text{x}'|\text{p}'\rangle$ which is just a diff eqn for $\langle \text{x}'|\text{p}'\rangle$

$\langle \text{x}'|\text{p}'\rangle = \text{N}e^{\left(\frac{\text{ip}' x'}{\hbar}\right)}$ where N is just a normalization. We can rewrite this more suggestively as

$\psi_{p'}(\text{x}') = \text{N}e^{\left(\frac{\text{ip}' x'}{\hbar}\right)}$ which says that the wave function for a momentum eigenstate in the position representation is just a bunch of sines and cosines - i.e. its a plane wave. Let's now find the normalization

this requires one of the ways to write down the delta function which is $2\pi\delta(\text{x-x}') = \int_{-\infty}^{\infty} e^{\text{ik}(x-x')}\,\text{dk}$ (See Liboff Appendix C)

$\delta(\text{x}'\text{-x}'') = \langle x'|x''\rangle = \int \text{dp}'\langle x'|p'\rangle\langle p'|x''\rangle = N^2 \int \text{dp}'\, e^{\left[\frac{\text{ip}'(x'-x'')}{\hbar}\right]} = N^2\, 2\pi\hbar\delta(\text{x}'\text{-x}'')$ so $N = \frac{1}{\sqrt{2\pi\hbar}}$ and finally

$\langle \text{x}'|\text{p}'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\left(\frac{\text{ip}' x'}{\hbar}\right)}$ and $\langle \text{p}'|\text{x}'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\left(\frac{-\text{ip}' x'}{\hbar}\right)}$

So lets now use this to switch between position and momentum basis

$\langle x'|\alpha\rangle = \int \text{dp}'\langle x'|p'\rangle\langle p'|\alpha\rangle \Longrightarrow \psi_\alpha(\text{x}') = \frac{1}{\sqrt{2\pi\hbar}}\int \text{dp}'\, e^{\left(\frac{\text{ip}' x'}{\hbar}\right)}\phi_\alpha(\text{p}')$ and the reverse

$\langle p'|\alpha\rangle = \int \text{dx}'\langle p'|x'\rangle\langle x'|\alpha\rangle \Longrightarrow \phi_\alpha(\text{p}') = \frac{1}{\sqrt{2\pi\hbar}}\int \text{dx}'\, e^{\left(\frac{-\text{ip}' x'}{\hbar}\right)}\psi_\alpha(\text{x}')$ so its just a fourier transform.

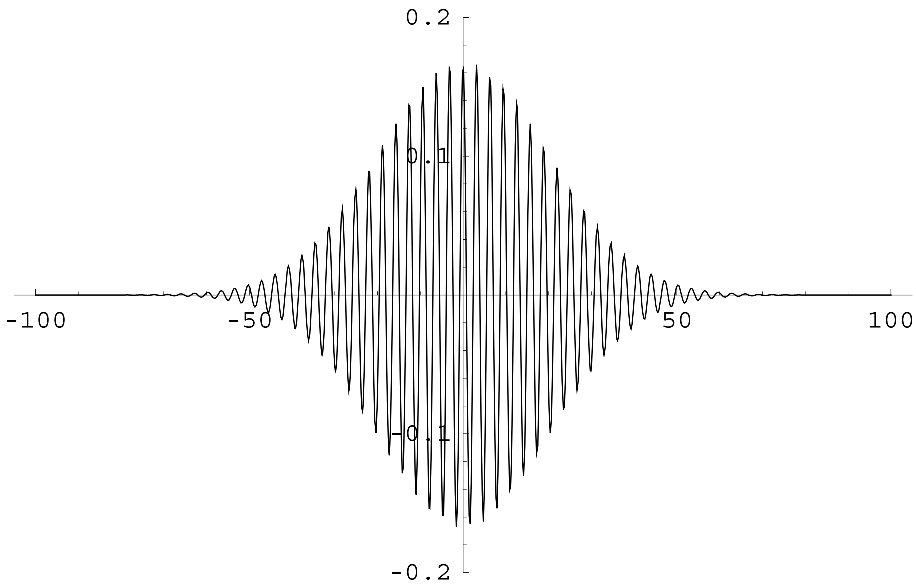
So lets do an example. Things are waves, so how can we think about a particle? Its a wave packet. Think about a musical note. Music (sound) comes to you in waves. But suppose someone plays a quick middle C on a flute - which gives a pretty pure tone with very few overtones. (Stacatto for the music folks)

Lets take a look at the function

$\langle x'|\alpha\rangle = \psi_\alpha(x') = \frac{1}{\pi^{\frac{1}{4}}\sqrt{d}}\, e^{\left[\text{ikx}-\frac{x^2}{2*d^2}\right]} = \frac{1}{\pi^{\frac{1}{4}}\sqrt{d}}\, e^{\text{ikx}} e^{\left[-\frac{x^2}{2*d^2}\right]}$ You can see that this is just a plane wave modulated by $e^{\left[-\frac{x^2}{2*d^2}\right]}$ which is a gaussian. The wave number is k. How does the wave look? Lets pick k=2 and d=20. The width of the gaussian envelope is 20, the wavelength is $\lambda = 2\pi/\text{k} = \pi$.

```
psi[x_, d_, k_] := 1/(Pi^(1/4) * Sqrt[d]) * Exp[I * k * x - x^2/(2 * d^2)]

Plot[Re[psi[x, 20., 2.]], {x, -100, 100}, PlotRange → {-.2, .2}]
```



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So you can see that the wavelength and envelope is as you would have expected.

First lets write this in the momentum representation

$\langle p'|\alpha\rangle = \phi_\alpha(p') = \int dx' \langle p'|x'\rangle \langle x'|\alpha\rangle = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\pi^{\frac{1}{4}}\sqrt{d}} \int dx' \, e^{\left(\frac{-ip'x'}{\hbar}\right)} e^{\left[ikx' - \frac{x'^2}{2*d^2}\right]}$ which after some work will be

$\langle p'|\alpha\rangle = \sqrt{\frac{d}{\hbar\sqrt{\pi}}} \, e^{\left[\frac{-(p'-\hbar k)^2 d^2}{2\hbar^2}\right]}$

We can figure out some stuff about this just for fun. How about the expectation value of x?

$\langle\hat{X}\rangle = \int\langle\alpha|x'\rangle x' \langle x'|\alpha\rangle \, dx' = \frac{1}{\sqrt{\pi}\,d} \int e^{\left(\frac{-x'^2}{d^2}\right)} x' \, dx' = 0$ makes sense

$\langle\hat{X}^2\rangle = \frac{1}{\sqrt{\pi}\,d} \int e^{\left(\frac{-x'^2}{d^2}\right)} x'^2 \, dx' = \frac{d^2}{2}$

$\left\langle(\Delta\hat{X})^2\right\rangle = \langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2 = \frac{d^2}{2}$

$\langle\hat{P}\rangle = \int\langle\alpha|x'\rangle \hat{P} \langle x'|\alpha\rangle \, dx' = \frac{1}{\sqrt{\pi}\,d} \int e^{\left[-ikx - \frac{x^2}{2*d^2}\right]} \frac{\hbar}{i} \frac{d}{dx} e^{\left[ikx - \frac{x^2}{2d^2}\right]} dx' = \frac{\hbar}{i} \frac{1}{\sqrt{\pi}\,d} \int dx \, e^{\left(\frac{-x'^2}{d^2}\right)} \left(ik - \frac{x}{d^2}\right) = \hbar k$

You can also do this in the p representation, but lets to the $\hat{P}^2$

$\langle \hat{P}^2 \rangle = \int \langle \alpha \,|p'\rangle\, \hat{P}^2 \,\langle p'\,|\alpha\rangle\, \mathrm{dp}' = \frac{d}{\hbar \sqrt{\pi}} \int e^{\left[\frac{-(p'-\hbar \mathrm{k})^2 d^2}{\hbar^2}\right]} p'^2\, \mathrm{dp}' \; = \frac{\hbar^2}{2 d^2} + \hbar^2 k^2$ so

$\left\langle \left(\Delta \hat{P}\right)^2 \right\rangle = \langle \hat{P}^2 \rangle - \langle \hat{P} \rangle^2 = \frac{\hbar^2}{2 d^2}$

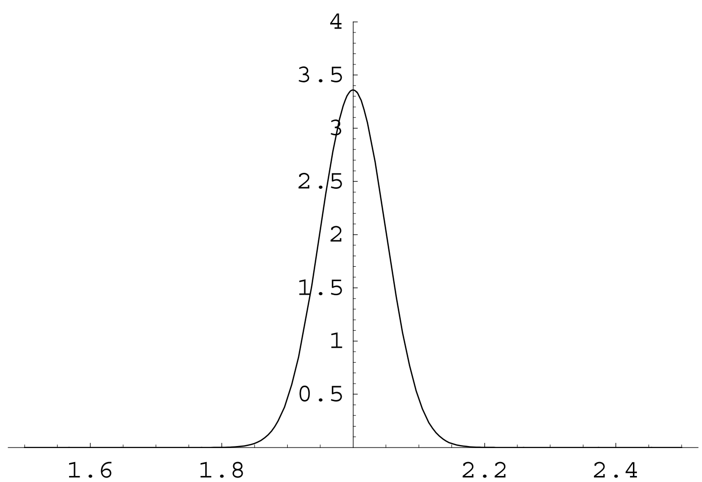
Now looking at Heisenberg

$\left\langle \left(\Delta \hat{X}\right)^2 \right\rangle \left\langle \left(\Delta \hat{P}\right)^2 \right\rangle = \frac{d^2}{2} \frac{\hbar^2}{2 d^2} = \frac{\hbar^2}{4}$ so $\left\langle \left(\Delta \hat{X}\right) \right\rangle \left\langle \left(\Delta \hat{P}\right) \right\rangle = \frac{\hbar}{2}$ so it is a state of minimum uncertainty.

Now lets look at the wave function of this thing in momentum representation.I will look at kprime since I dont want to have $\hbar$ floating around to mess the plots up.

```
phi[kprime_, d_, k_] := Sqrt[d]/Pi^(1/4) * Exp[-(kprime - k)^2 d^2/2]

Plot[Re[phi[kprime, 20., 2.]], {kprime, 1.5, 2.5}, PlotRange → {0., 4.}]
```



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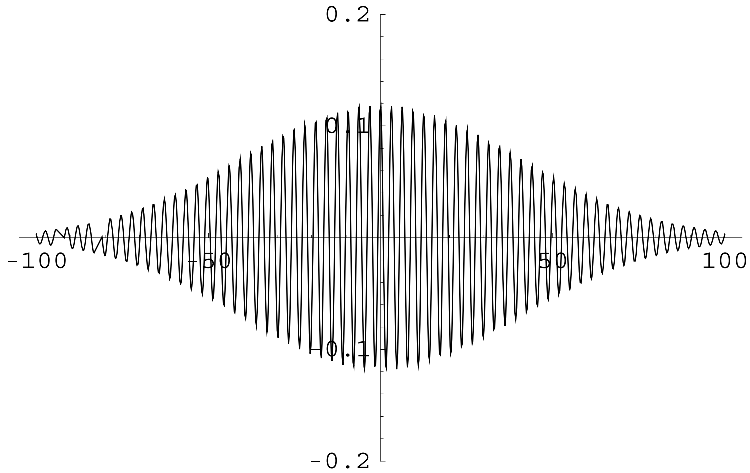
Remember the x axis is now p (actually kprime). Its a nice distribution around k=2 (which is what we expected since that is what I chose) Its width is 1/d

Now lets see if we let d get larger.

```
Plot[Re[psi[x, 40., 2.]], {x, −100, 100},  PlotRange → {−.2, .2}]
Plot[Re[phi[kprime, 40., 2.]], {kprime, 1.0, 3.0}, PlotRange → {0., 6.}]
```



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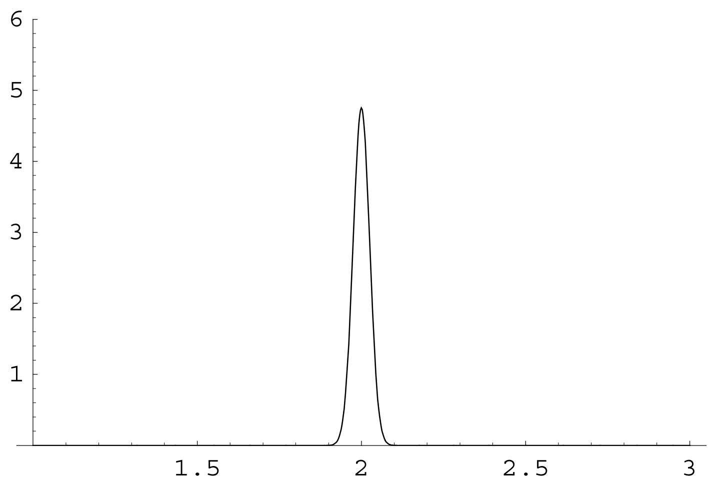

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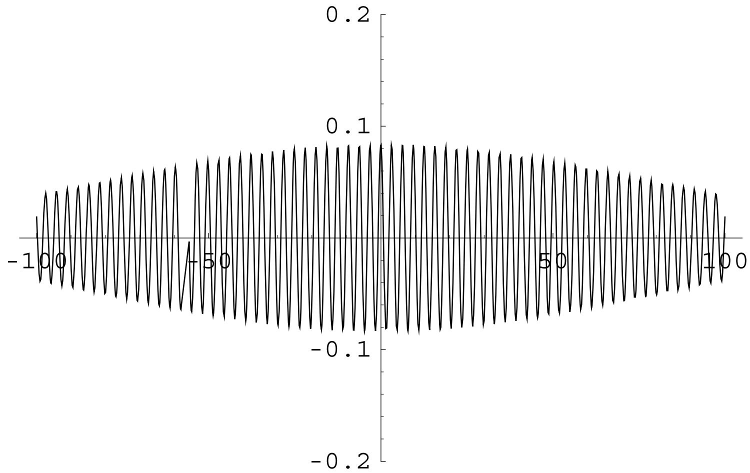
```
Plot[Re[psi[x, 80., 2.]], {x, -100, 100}, PlotRange → {-.2, .2}]
Plot[Re[phi[kprime, 80., 2.]], {kprime, 1.5, 2.5}, PlotRange → {0., 8.}]
```



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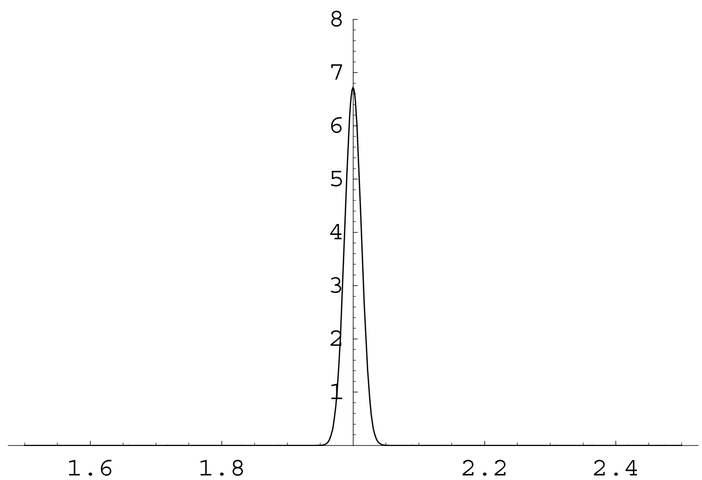

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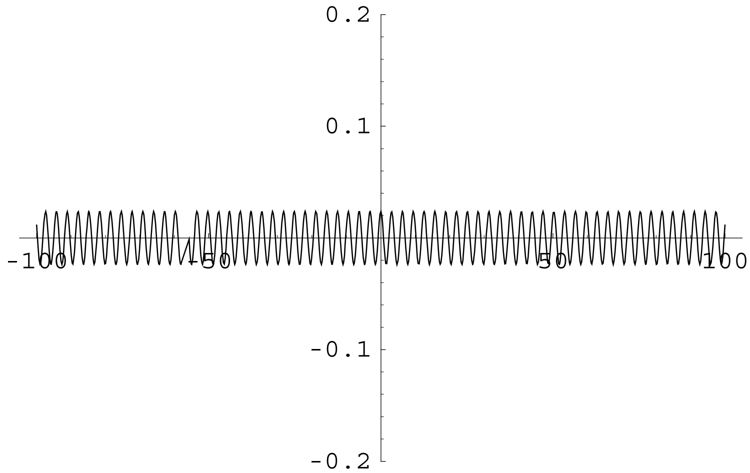
We see that the position distribution gets wider, and the momentum distribution gets narrower. This is what we expect from heisenberg.

```
Plot[Re[psi[x, 1000., 2.]], {x, -100, 100}, PlotRange → {-.2, .2}]
Plot[Re[phi[kprime, 1000., 2.]], {kprime, 1.0, 3.0}, PlotRange → {0., 25.}]
```



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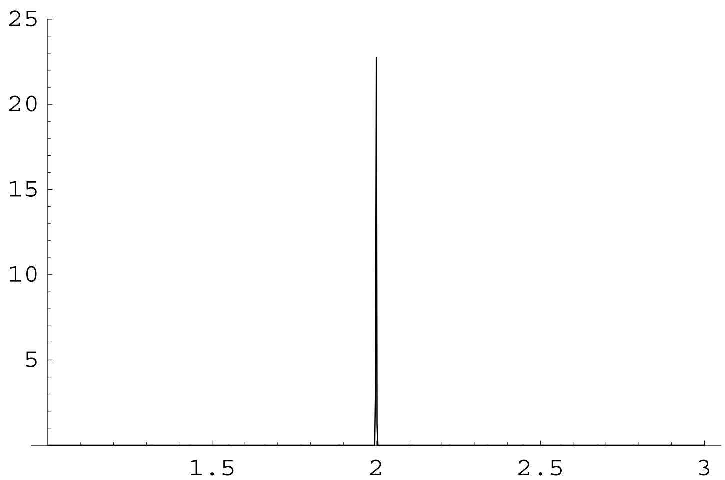

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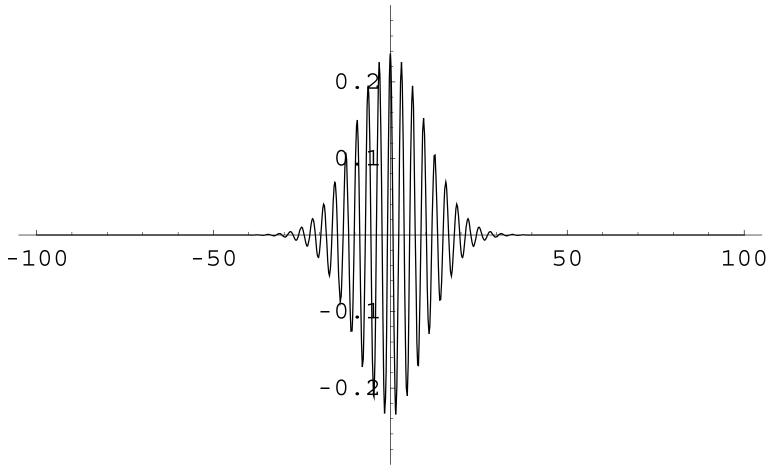
Eventually the position distribution gets very wide and the momentum distribution becomes almost a delta function.

Now lets try going the other way and make d small

```
Plot[Re[psi[x, 10., 2.]], {x, -100, 100},  PlotRange → {-.3, .3}]
Plot[Re[phi[kprime, 10., 2.]], {kprime, 1.0, 3.0}, PlotRange → {0., 4.}]
```



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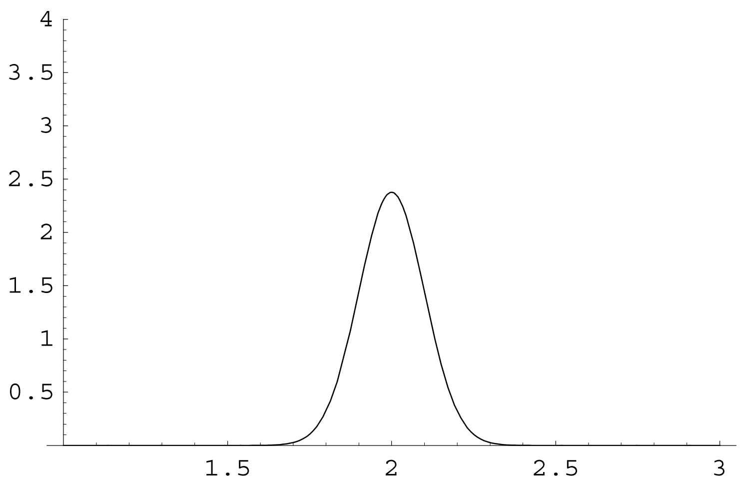

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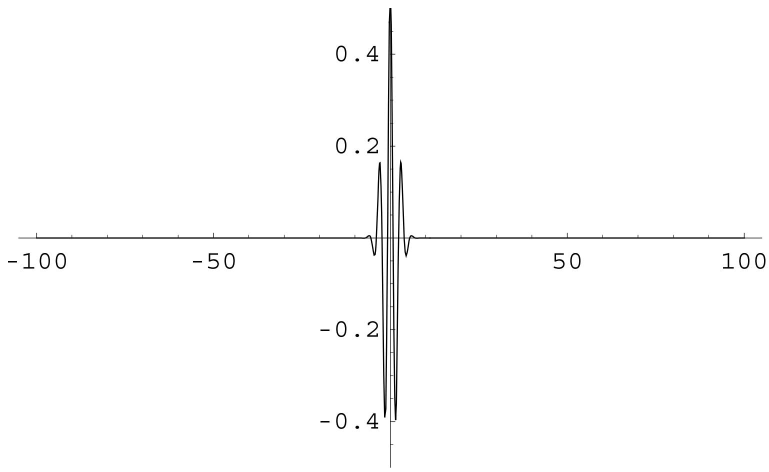
```
Plot[Re[psi[x, 2., 2.]], {x, −100, 100}, PlotRange → {−.5, .5}]
Plot[Re[phi[kprime, 2., 2.]], {kprime, 1.0, 3.0}, PlotRange → {0., 4.}]
```



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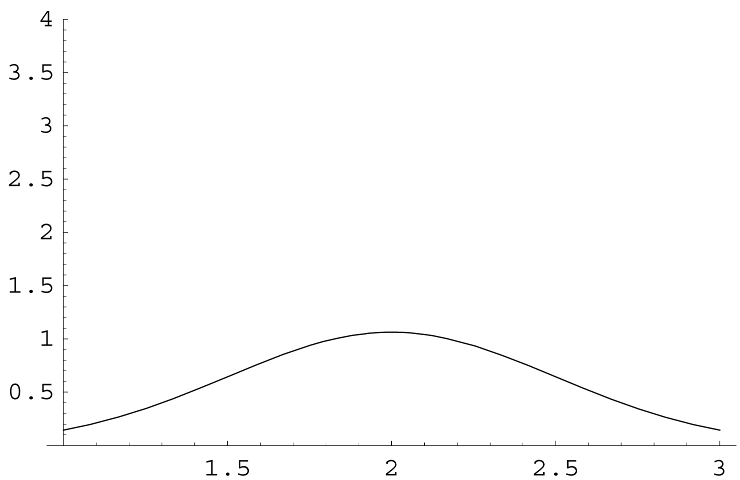

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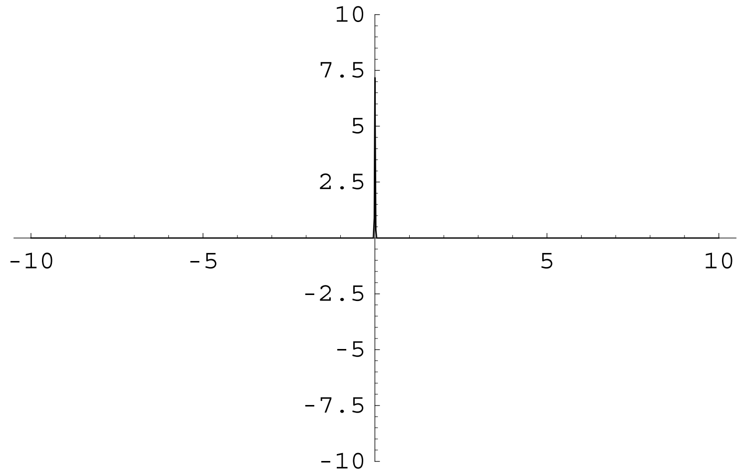
```
Plot[Re[psi[x, .01, 2.]], {x, −10, 10}, PlotRange → {−10, 10.}]
Plot[Re[phi[kprime, .01, 2.]], {kprime, 1.0, 3.0}, PlotRange → {0., .5}]
```



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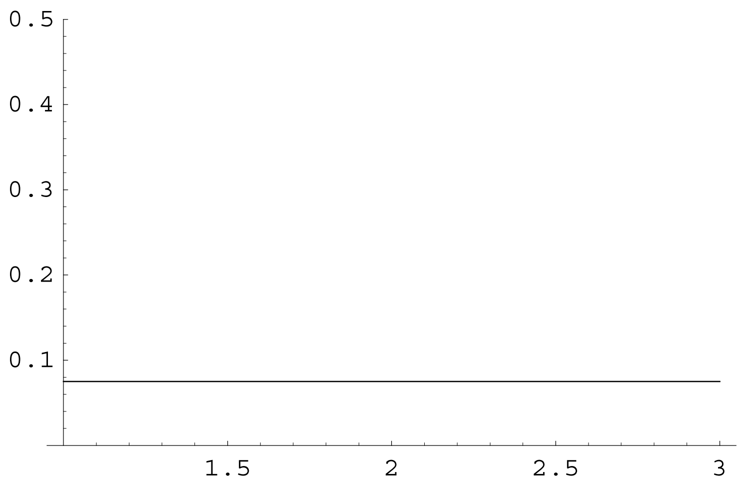

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Eventually the position distribution becomes localized at one value, but it covers all momenta. So what we have made is a very localized wave packet - almost at a single point. But the momentum is totally unconstrained.

So you can never beat the Heisenberg Uncertainty principle. If you make gains in one, you loose in the other.