Example: A Gaussian wave packet

Consider the following normalized wave-function:

$$\psi(x) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} e^{-\frac{x^2}{4\sigma_x^2}} = \alpha e^{-\beta^2 x^2} \tag{2.1}$$

where:

$$\alpha \equiv \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4}, \qquad \beta^2 \equiv \frac{1}{4\sigma_x^2} \tag{2.2}$$

This represents a wave packet with $\langle x \rangle = 0$ and a standard deviation of σ_x. The Fourier transform is:

$$\phi(k) = \frac{\alpha}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{(-\beta^2 x^2 - ikx)}\, dx \tag{2.3}$$

We can use the "Completing the square" method to do this integral : in the general case

$$\int_{-\infty}^{\infty} e^{-(a^2x^2+bx)} dx \tag{2.4}$$

let $y = (ax + b/2a)$: then,

$$y^2 - \frac{b^2}{4a^2} = a^2x^2 + bx \tag{2.5}$$

and

$$\frac{1}{a} dy = dx \tag{2.6}$$

$$\int_{-\infty}^{\infty} e^{-(a^2x^2+bx)} dx = \frac{e^{b^2/(4a^2)}}{a} \int_{-\infty}^{\infty} e^{-y^2} dy \tag{2.7}$$

$$= \frac{e^{b^2/(4a^2)}}{a} \sqrt{\pi} \tag{2.8}$$

In our case $a = \beta$ and $b = ik$; substituting,

$$\phi(k) = \frac{\alpha}{\beta\sqrt{2}} e^{-\frac{k^2}{4\beta^2}} \tag{2.9}$$

Substituting in the definition of α:

$$\phi(k) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} \frac{1}{\beta\sqrt{2}} e^{-\frac{k^2}{4\beta^2}} \tag{2.10}$$

Expressing σ_x in terms of β:

$$\phi(k) = \left(\frac{2\beta^2}{\pi}\right)^{1/4} \frac{1}{\beta\sqrt{2}} e^{-\frac{k^2}{4\beta^2}} = \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{-\frac{k^2}{4\beta^2}} \tag{2.11}$$

This is exactly the same form that we started with for $\psi(x)$. The square of the distribution $|\phi(k)|^2$ is normalized over the region of k running from $-\infty$ to ∞, so it probably is not too difficult to imagine that it is the probability distribution for values of k. In fact the function plays the same role as the c_n's did in the infinite square well problem. The probability distribution is a Gaussian function with standard deviation $\sigma_k = \beta = 1/(2\sigma_x)$. Thus:

$$\sigma_k \sigma_x = \frac{1}{2} \tag{2.12}$$

If we use $p = \hbar k$, we obtain:

$$\sigma_p \sigma_x = \frac{\hbar}{2} \tag{2.13}$$

which is the minimum value allowed by the Heisenberg uncertainty principle.

We can now use this as the transform of the wave-function to obtain at $t = t$:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx}\, e^{-i\frac{\hbar k^2}{2m}t}\, dk = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\frac{(k)^2}{4\beta^2}}\, e^{ikx}\, e^{-i\frac{\hbar k^2}{2m}t}\, dk \tag{2.14}$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\left[k^2\left(\frac{1}{4\beta^2} + i\frac{\hbar}{2m}t\right) - ikx\right]}\, dk \tag{2.15}$$

We can use "Completing the square" here with $a = \sqrt{\left(\frac{1}{4\beta^2} + i\frac{\hbar}{2m}t\right)}$ and $b = -ix$. After substituting for β^2 we get,

$$\Psi(x,t) = \left(\frac{1}{2\pi\sigma_0^2}\right)^{1/4} \frac{1}{\sqrt{\left(1 + \frac{i\hbar t}{2m\sigma_0^2}\right)}} \exp\left[\frac{-x^2}{4\sigma_0^2(1 + i\hbar t/(2m\sigma_0^2))}\right] \tag{2.16}$$

For this wave-function $\langle x \rangle = 0$, and $\langle p \rangle = 0$. We can put the particle into uniform motion by modifying $\phi(k)$ to shift the centroid to a non-zero value:

$$\phi(k) = \left(\frac{2\beta^2}{\pi}\right)^{1/4} \frac{1}{\beta\sqrt{2}} e^{-\frac{(k-k_0)^2}{4\beta^2}} = \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{-\frac{(k-k_0)^2}{4\beta^2}} \tag{2.17}$$

Again, substituting this $\phi(k)$ in the equation for $\Psi(x,t)$ and integrating, we get:

$$\Psi(x,t) = \left[(2\pi\sigma_0^2)^{1/2}\left(1+\frac{i\hbar t}{2m\sigma_0^2}\right)\right]^{-1/2}$$

$$\times\exp\left[\frac{-(x-p_0t/m)^2}{4\sigma_0^2(1+i\hbar t/(2m\sigma_0^2))}\right]\times\exp\left[\frac{ip_0}{\hbar}\left(x-\frac{p_0t}{2m}\right)\right] \tag{2.18}$$

The probability distribution at $t=0$ is:

$$P(x,0) = |\psi^*\psi| = \frac{e^{-x^2/2\sigma_0^2}}{(2\pi\sigma_0^2)^{1/2}} \tag{2.19}$$

which is the familiar normalized Gaussian distribution with $\langle x\rangle = 0$ and where $\sigma_x = \sigma_0$ is the s.d. in x. To calculate the expectation value for the momentum at $t=0$, first calculate the spatial derivative of the wave function, eqn. 2.18

$$\frac{\partial}{\partial x}\Psi = \left[\frac{ip_0}{\hbar} - \frac{x}{2\sigma_0^2}\right]\Psi$$

so

$$p\Psi = \frac{\hbar}{i}\frac{\partial\Psi}{\partial x} = \left[p_0 + i\hbar\frac{x}{2\sigma_0^2}\right]\Psi$$

From this equation we can read off that:

$$\langle p\rangle = p_0 + i\hbar\frac{\langle x\rangle}{2\sigma_0^2} = p_0 \tag{2.20}$$

To calculate $\langle p^2\rangle$ at time $t=0$:

$$p^2\Psi = -\hbar^2\frac{\partial^2\Psi}{\partial x^2} = -\hbar^2\left(\left[\frac{ip_0}{\hbar} - \frac{x}{2\sigma_0^2}\right]^2 - \frac{1}{2\sigma_0^2}\right)\Psi \tag{2.21}$$

$$p^2\Psi = -\hbar^2\left(-\frac{p_0^2}{\hbar^2} - 2\frac{ip_0x}{2\hbar\sigma_0^2} + \frac{x^2}{4\sigma_0^4} - \frac{1}{2\sigma_0^2}\right)\Psi \tag{2.22}$$

$$p^2\Psi = \left(p_0^2 + 2\frac{i\hbar p_0x}{2\sigma_0^2} - \frac{\hbar^2x^2}{4\sigma_0^4} + \frac{\hbar^2}{2\sigma_0^2}\right)\Psi \tag{2.23}$$

With this result, we immediately obtain without any integrations:

$$\langle p^2\rangle = p_0^2 + 2\frac{i\hbar p_0\langle x\rangle}{2\sigma_0^2} - \frac{\hbar^2\langle x^2\rangle}{4\sigma_0^4} + \frac{\hbar^2}{2\sigma_0^2} = p_0^2 - \frac{\hbar^2\langle x^2\rangle}{4\sigma_0^4} + \frac{\hbar^2}{2\sigma_0^2} \tag{2.24}$$

Recalling that $\langle x^2 \rangle = \sigma_x^2 = \sigma_0^2$:

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{4\sigma_x^2} \tag{2.25}$$

so:

$$\sigma_p \sigma_x = \frac{\hbar}{2} \tag{2.26}$$

At $t = 0$ the wave function satisfies the minimum uncertainty allowed by the Heisenberg Uncertainty Principle.

Now let us see how this wave function evolves with time. Returning to the time dependent function, eqn. 2.18, let us write it as

$$\Psi(x,t) = \frac{A}{\sqrt{s}} e^{-\frac{(x-vt)^2}{4s}} e^{\frac{ip_0}{\hbar}\left(x - \frac{vt}{2}\right)} = N(t) e^{-\frac{(x-vt)^2}{4s}} e^{\frac{ip_0}{\hbar}\left(x - \frac{vt}{2}\right)}$$

where

$$s \equiv \sigma_0^2 + \frac{i\hbar t}{2m}$$
$$A \equiv (2\pi\sigma_0^2)^{-1/4}\sigma_0$$
$$v \equiv \frac{p_0}{m}$$

and where $N(t)$ is the normalization factor. The complex conjugate of the wave function is

$$\Psi(x,t)^* = N^* e^{-\frac{(x-vt)^2}{4s^*}} e^{\frac{-ip_0}{\hbar}\left(x - \frac{vt}{2}\right)}$$

Their product provides the probability distribution,

$$P(x,t) = \Psi^*\Psi = |N|^2 e^{-\frac{(x-vt)^2}{4}\left(\frac{1}{s} + \frac{1}{s^*}\right)} = |N|^2(t) e^{-\frac{(x-vt)^2}{2\sigma_x(t)^2}}$$

The probability distribution is a Gaussian for any time centered at

$$\langle x(t) \rangle = vt$$

The standard deviation in the spatial distribution is given by $\sigma_x(t)$, which is given by

$$\frac{1}{\sigma_x(t)^2} = \frac{1}{2}\left(\frac{1}{s} + \frac{1}{s^*}\right) = \frac{s + s^*}{2ss^*}$$
$$\sigma_x^2 = \frac{2ss^*}{s + s^*}$$

Now

$$s + s^* = 2\sigma_0^2$$

and

$$ss^* = \sigma_0^4 + \frac{\hbar^2 t^2}{4m^2}$$

so

$$\sigma_x^2 = \frac{\sigma_0^4 + \frac{\hbar^2 t^2}{4m^2}}{\sigma_0^2} = \sigma_0^2 \left(1 + \frac{\hbar^2 t^2}{4m^2 \sigma_0^4}\right)$$

$$\sigma_x(t) = \sigma_0 \sqrt{1 + \frac{\hbar^2 t^2}{4m^2 \sigma_0^4}}$$

The wave-packet spreads out as time increases, and the particle becomes less and less localized. The tighter the initial localization, i.e. the smaller the value of σ_0, the more rapidly the wave function spreads out.

It is straight-forward to show that the momentum distribution is constant in time: $\langle p(t)\rangle = p_0$ and $\sigma_p(t) = \sigma_p(t=0)$. We need the derivatives of the wave-function;

$$\frac{\partial \Psi}{\partial x} = -\left[\frac{x - vt}{2s} - \frac{ip_0}{\hbar}\right]\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \left(\left[\frac{x - vt}{2s} - \frac{ip_0}{\hbar}\right]^2 - \frac{1}{2s}\right)\Psi$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \left(\frac{x^2 - 2xvt + v^2t^2}{4s^2} - \frac{ip_0(x - vt)}{\hbar s} - \frac{p_0^2}{\hbar^2} - \frac{1}{2s}\right)\Psi$$

It follows that

$$\langle p\rangle = -\frac{\hbar}{i}\left[\frac{\langle x\rangle - vt}{2s} - \frac{ip_0}{\hbar}\right] = -\frac{\hbar}{i}\left[-\frac{ip_0}{\hbar}\right] = p_0$$

and

$$\langle p^2\rangle = -\hbar^2\left(\frac{\langle x^2\rangle - 2vt\langle x\rangle + v^2t^2}{4s^2} - \frac{ip_0(\langle x\rangle - vt)}{\hbar s} - \frac{p_0^2}{\hbar^2} - \frac{1}{2s}\right)$$

Using $\langle x\rangle = vt$, this reduces to

$$\langle p^2\rangle = -\hbar^2\left(\frac{\langle x^2\rangle - 2\langle x\rangle^2 + \langle x\rangle^2}{4s^2} - \frac{1}{2s}\right) + p_0^2$$

so that

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 == -\hbar^2 \left(\frac{\langle x^2 \rangle - \langle x \rangle^2}{4s^2} - \frac{1}{2s} \right) = \frac{\hbar^2}{2s} \left(1 - \frac{\sigma_x^2}{2s} \right)$$

$$= \frac{\hbar^2}{2s} \left(1 - \frac{2ss^*}{2s(s+s^*)} \right) = \frac{\hbar^2}{2s} \left(1 - \frac{s^*}{(s+s^*)} \right) = \frac{\hbar^2}{2s} \left(\frac{s}{(s+s^*)} \right) = \frac{\hbar^2}{2(s+s^*)}$$

$$\sigma_p^2 = \frac{\hbar^2}{4\sigma_0^2}$$

so

$$\sigma_p(t) = \sigma_p(t=0)$$

The expectation value of the momentum and its standard deviation remain constant. The product of the two uncertainties grows with time. A **free** particle that satisfies the minimum requirement of the uncertainty principle at time $t = 0$ will not do so for later times.

2.0.1 Group Velocity

Another problem that we noticed with the single energy wave solutions of the free