0.1 Motion in 1-dimensional space

To present a particle moving along the real axis, we define a Hilbert space having as its regular vectors $|f\rangle$ the complex-valued, continuous, and square-integrable functions on the real numbers:

$$f : \mathbb{R} \to \mathbb{C} \qquad\qquad \int_{-\infty}^{\infty} f^*(x) f(x) dx < \infty$$

We do, however, allow our basis to violate the requirement of square-integrability, giving us the pseudo-bases of

$$X \mid x \rangle = x \mid x \rangle$$

or

$$P \mid p \rangle = p \mid p \rangle$$

We can project our waveform ψ onto a particular basis like so

$$\langle x \mid \psi \rangle = \psi(x)$$

$$\langle p \mid \psi \rangle = \tilde{\psi}(p)$$

If we try to get the x projection of canonical momentum, then

$$\langle x \mid P \mid \psi \rangle = \int dx' \langle x \mid P \mid x' \rangle \langle x' \mid \psi \rangle$$

$$= \int \frac{\hbar}{i} \delta'(x - x') \psi(x') dx'$$

$$= \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x)$$

We remind ourselves:

$$\langle x \mid p \rangle = \Phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$$

$$\langle p \mid x \rangle = \psi_x(p) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{-ipx}{\hbar}}$$

The connection between $\psi(x)$ and $\tilde{\psi}(p)$ is theFourier transform

$$\tilde{\psi}(p) = \langle p \mid \psi \rangle = \int_{-\infty}^{\infty} \langle p \mid x' \rangle \langle x' \mid \psi \rangle dx' = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{-ipx'}{\hbar}} \psi(x') dx'$$

Like-wise

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \tilde{\psi}(p) dp$$

Given the hamiltonian for a free particle with no forces on it:

$$H = \frac{p^2}{2m}$$

We want to find a basis of eigenvectors

$$H \mid \psi_i\rangle = E_i \mid \psi_i\rangle$$

$$\psi_i(t) = \psi_i(0) e^{\frac{-iE_i t}{\hbar}}$$

Apparently, our p-basis fils the bill:

$$H \mid p\rangle = \frac{p^2}{2m} \mid p\rangle$$

$$E = \frac{p^2}{2m}$$

Each eigenvalue is twice degenerate, because $\mid p\rangle$ and $\mid -p\rangle$ give you the same value. Any linear combination of degenerate eigenstates is also an eigenstate of the same eigenvalue. That is,

$$\frac{1}{\sqrt{2}} \mid p\rangle + \frac{1}{\sqrt{2}} \mid -p\rangle$$

is also an eigenstate.

0.2 Propagator

Given that we know $\psi(0)$ how to we find $\psi(t)$?

$$\mid \psi_0\rangle = \int dp \langle p \mid \psi(0)\rangle \mid p\rangle \Rightarrow \mid \psi(t)\rangle = \int dp \langle p \mid \psi(0)\rangle e^{\frac{-ip^2 t}{2m\hbar}} \mid p\rangle$$

$$\mid \psi(t)\rangle = U(t) \mid \psi(0)\rangle = \left(\int dp \mid p\rangle \langle p \mid e^{\frac{-ip^2 t}{2m\hbar}} \right) \mid \psi(0)\rangle$$

The expression in parentheses is the unitary propagator in time, the operator $U(t)$.

We can use this propagator to answer the following question: If we know the wave function at every point for the initial time $t = 0$, $\psi(x, 0)$, how can we "propagate" this information to the wave function $\psi(x, t)$ at time t? We are looking for the propagator in x-space, $U(x, t; x', t = 0)$. You can think of this as an operator that calculates the contribution coming to the point x from the initial value of the wave function at x', after some time t has elapsed. (Think of electromagnetic waves as an example: The value at some point in space and time t is the linear superposition of all values at earlier times that have traveled to this point.)

$$\psi(x, t) = \langle x \mid U(t) \mid \psi(0) \rangle = \int dx' \langle x \mid U(t) \mid x' \rangle \langle x' \mid \mid \psi(0) \rangle = \int dx' U(x, t; x', 0) \psi(x', 0)$$

Plugging in, we get

$$\langle x \mid U(t) \mid x' \rangle = \int dp \langle x \mid p \rangle e^{\frac{-ip^2 t}{2m\hbar}} \langle p \mid x' \rangle = \frac{1}{2\pi\hbar} \int e^{i\frac{px}{\hbar}} e^{\frac{-ip^2 t}{2m\hbar}} e^{\frac{-ipx'}{\hbar}} dp$$

Recall from Appendix A2 in *Shankar*

$$\int_{-\infty}^{\infty} e^{-ay^2 + by + c} dy = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}} e^{c}$$

Here, $a = it/2m\hbar$ and $b = i(x - x')/\hbar$ and thus

$$U(x, t; x') = \sqrt{\frac{m}{2\pi\hbar it}} e^{-\frac{m}{2\hbar it}(x - x')^2}$$

and

$$\psi(x, t) = \int U(x, t; x') \psi(x', t = 0) dx'.$$

Note that, taken literally, $U(x, t; x', 0)$ would be the wave function of a particle at time t that was in the state $|x'\rangle$ at time $t = 0$. At first glance one might think that the exponential guarantees that one can find this particle still nearby at later times; however, if you take the absolute square, you find that the probability to find the particle *anywhere*, even only a split second later, is the same - whether right were it started or behind the moon. This is a consequence of the fact that the momentum in this case is completely undetermined (and can thus be any arbitrary value, so any arbitrary distance can be travelled in an arbitrarily short time). Formally, it's a consequence of the fact that $|x\rangle$ is not a proper vector in the Hilbert space and therefore cannot represent a real state of a real particle.

0.3 Gaussian Wave Packets

One cannot prepare a state with perfect position and momentum, so instead you prepare a Gaussian around a point x_0 with an average momentum p_0:

$$\psi(x, t = 0) = \sqrt{\frac{1}{\sqrt{2\pi}\sigma}} e^{\frac{ip_0 x}{\hbar}} e^{\frac{-(x-x_0)^2}{4\sigma^2}}$$

$$Prob(x...x + dx) = |\psi(x)|^2 dx; \ |\psi(x)|^2 = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(x-x_0)^2}{2\sigma^2}}$$

This is the usual Gaussian probability distribution with mean $< x >= x_0$ and standard deviation σ.

In momentum space:

$$\tilde{\psi}(p, t = 0) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{\frac{-ipx}{\hbar}} \psi(x) dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}\sigma} \frac{1}{(2\pi)^{\frac{1}{4}}} \int e^{-\frac{1}{4\sigma^2}(x^2 - 2x_0 x + x_0^2) + \frac{i(p_0 - p)}{\hbar} x} dx$$

So, $a = \frac{1}{4\sigma^2}$, $b = \frac{x_0}{2\sigma^2} + \frac{i(p_0 - p)}{\hbar}$ and $c = -\frac{x_0^2}{4\sigma^2}$. Therefore,

$$\tilde{\psi}(p, t = 0) = \sqrt{\pi 4\sigma^2} \frac{1}{\sqrt{2\pi\hbar}\sigma} \frac{1}{(2\pi)^{\frac{1}{4}}} e^{\frac{b^2}{4a}} e^c = \sqrt{\frac{2\sigma}{\sqrt{2\pi}\hbar}} e^{-\frac{(p_0-p)^2}{\hbar^2}\sigma^2 + \frac{i(p_0-p)x_0}{\hbar}}$$

$$= \frac{1}{\sqrt{\sqrt{2\pi}\frac{\hbar}{2\sigma}}} e^{-\frac{(p-p_0)^2}{4\frac{\hbar^2}{4\sigma^2}}} e^{-\frac{i(p-p_0)x_0}{\hbar}}$$

$$|\tilde{\psi}(p)|^2 = \frac{1}{\sqrt{2\pi}\frac{\hbar}{2\sigma}} e^{-\frac{(p-p_0)^2}{2\frac{\hbar^2}{4\sigma^2}}}$$

$$\langle p \rangle = p_0$$

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

Thus

$$\Delta x \Delta p = \frac{\hbar}{2}$$

We find that the Gaussian wave packet has the smallest product for the uncertainties of position and momentum that is allowed by the Heisenberg

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uncertainty relationship. It is the best possible approximation to a "localized" particle moving along the x-axis with definite momentum. The width in either position or momentum space can be chosen arbitrarily, but the other one will then be inversely proportional. Unfortunately, as we will see now, the Gaussian wave packet doesn't remain localized in x-space (although it has constant width in momentum space).

Let's find $\psi(x, t)$ using the propagator $U(x, t; x', 0)$ introduced above.

$$\psi(x, t) = \sqrt{\frac{m}{2\pi\hbar it}} \frac{1}{\sqrt{\sigma}(2\pi)^{\frac{1}{4}}} \int e^{\frac{ip_0 x'}{\hbar}} e^{-\frac{1}{4\sigma^2}(x'-x_0)^2} e^{-\frac{m}{2\hbar it}(x^2-2xx'+x'^2)} dx'$$

Here, $a = \frac{1}{4\sigma^2} + \frac{m}{2\hbar it}$, $b = \frac{ip_0}{\hbar} + \frac{x_0}{2\sigma^2} + \frac{mx}{\hbar it}$ and $c = -\frac{x_0^2}{4\sigma^2} - \frac{mx^2}{2\hbar it}$. Therefore,

$$\frac{b^2}{4a} = \left(\frac{x_0}{2\sigma^2} + \frac{i}{\hbar}(p_0 - \frac{mx}{t}) \right)^2 \left(\frac{1}{\sigma^2} + \frac{2m}{\hbar it} \right)^{-1} \tag{1}$$

and

$$\psi(x, t) = \sqrt{\frac{m}{2\pi\hbar ti\sigma}} \frac{1}{(2\pi)^{\frac{1}{4}}} \sqrt{\frac{\pi}{\frac{1}{4\sigma^2} - \frac{im}{2\hbar t}}} e^{\frac{-2p_0\sigma^2(p_0 t - 2mx) + i\hbar(m(x-x_0)^2 + 2p_0 x_0 t)}{2\hbar(\hbar t - 2im\sigma^2)}}.$$

This gives us

$$\psi(x, t) = \sqrt{\frac{m}{2\pi\hbar ti\sigma}} \frac{1}{(2\pi)^{\frac{1}{4}}} \sqrt{\frac{\pi}{\frac{1}{4\sigma^2} - \frac{im}{2\hbar t}}} e^{-\frac{(p_0 t/m + x_0 - x)^2}{4(\sigma^2 + (\hbar/2\sigma)^2 t^2/m^2)}} e^{i\Im\left(\frac{b^2}{2a} + c\right)}$$

where I expanded the exponent to collect its real and imaginary parts.

Let the coefficient in front of the expontential be represented by ζ; then

$$|\psi(x, t)|^2 = \zeta^* \zeta e^{-\frac{(x - (p_0 t/m + x_0))^2}{2(\sigma^2 + \sigma_p^2 t^2/m^2)}} = \frac{1}{\sqrt{2\pi}\sqrt{(\sigma^2 + \sigma_p^2 t^2/m^2)}} e^{-\frac{(x - (p_0 t/m + x_0))^2}{2(\sigma^2 + \sigma_p^2 t^2/m^2)}}$$

This is a new Gaussian probability distribution with a mean of

$$\langle x \rangle = \frac{p_0}{m} t + x_0$$

and a width of

$$\sigma_x^2 = \sigma^2 + \frac{\sigma_p^2}{m^2} t^2$$

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Over time, the center of the wave packet moves from x_0 with constant velocity p_0/m in x-direction. At the same time, its width in x spreads out because of the additional widening due to the momentum uncertainty. The first aspect of this motion agrees with the correspondence principle, which says that Classical Mechanics can be retrieved as the average behavior of expectation values in Quantum Mechanics; however, the fully Classical description is not correct since it misses the initial width and further spreading of the wave packet. On the other hand, in the limit of large masses, it takes centuries for any appreciable spreading, so in this limit Classical Mechanics becomes applicable.