Gaussian Wave Packets

The Gaussian wave packet initial state is one of the few states for which both the $\{|x\rangle\}$ and $\{|p\rangle\}$ basis representations are simple analytic functions and for which the time evolution in either representation can be calculated in closed analytic form. It thus serves as an excellent example to get some intuition about the Schrödinger equation.

We define the $\{|x\rangle\}$ representation of the initial state to be

$$\psi_x(x, t=0) = \langle x\,|\psi(0)\,\rangle = \left(\frac{1}{2\,\pi\,\sigma_x^2}\right)^{1/4} e^{\frac{i}{\hbar}\,p_0\,x}\, e^{-\frac{x^2}{4\,\sigma_x^2}} \tag{5.10}$$

The relation between our σ_x and Shankar's Δ_x is $\Delta_x = \sigma_x\sqrt{2}$. As we shall see, we choose to write in terms of σ_x because $\langle(\Delta X)^2\rangle = \sigma_x^2$.

The Free Particle (cont.)

Before doing the time evolution, let's better understand the initial state. First, the symmetry of $\langle x \,|\psi(0)\,\rangle$ in x implies $\langle X \rangle_{t=0} = 0$, as follows:

$$\begin{aligned}
\langle X \rangle_{t=0} &= \langle \psi(0)\,| X \,|\psi(0)\,\rangle = \int_{-\infty}^{\infty} dx\, \langle \psi(0)\,| X \,| x\,\rangle \langle x \,|\psi(0)\,\rangle \\
&= \int_{-\infty}^{\infty} dx\, \langle \psi(0)\,| x\,\rangle\, x\, \langle x \,|\psi(0)\,\rangle \\
&= \int_{-\infty}^{\infty} dx\, x \left(\frac{1}{2\,\pi\,\sigma_x^2} \right)^{1/2} e^{-\frac{x^2}{2\,\sigma_x^2}} = 0
\end{aligned} \tag{5.11}$$

because the integrand is odd.

Second, we can calculate the initial variance $\langle (\Delta X)^2 \rangle_{t=0}$:

$$\langle (\Delta X)^2 \rangle_{t=0} = \int_{-\infty}^{\infty} dx\, \left(x^2 - \langle X \rangle_{t=0}^2\right) \left(\frac{1}{2\,\pi\,\sigma_x^2} \right)^{1/2} e^{-\frac{x^2}{2\,\sigma_x^2}} = \sigma_x^2 \tag{5.12}$$

where we have skipped a few steps that are similar to what we did above for $\langle X \rangle_{t=0}$ and we did the final step using the Gaussian integral formulae from Shankar and the fact that $\langle X \rangle_{t=0} = 0$.

The Free Particle (cont.)

We calculate the $\{|p\,\rangle\}$-basis representation of $|\psi(0)\,\rangle$ so that calculation of $\langle P \rangle_{t=0}$ and $\langle (\Delta P)^2 \rangle_{t=0}$ are easy (by contrast, Shankar Example 4.2.4 does this in the $\{|x\,\rangle\}$ basis):

$$\psi_p(p, t=0) = \langle p\,|\psi(0)\,\rangle = \int_{-\infty}^{\infty} dx\,\langle p\,|x\,\rangle\langle x\,|\psi(0)\,\rangle$$
$$= \frac{1}{\sqrt{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} dx\, e^{-\frac{i}{\hbar}\,p\,x} \left(\frac{1}{2\,\pi\,\sigma_x^2}\right)^{1/4} e^{\frac{i}{\hbar}\,p_0\,x}\, e^{-\frac{x^2}{4\,\sigma_x^2}}$$
$$= \left(\frac{1}{2\,\pi\,\sigma_p^2}\right)^{1/4} e^{-\frac{(p-p_0)^2}{4\,\sigma_p^2}} \tag{5.13}$$

where the $\frac{1}{\sqrt{\hbar}}$ comes from the normalization $|p\,\rangle = \frac{1}{\sqrt{\hbar}}\,|k\,\rangle$, where $\sigma_p \equiv \frac{\hbar}{2\,\sigma_x}$, and the final step is done by completing the square in the argument of the exponential and using the usual Gaussian integral $\int_{-\infty}^{\infty} du\, e^{-u^2} = \sqrt{\pi}$. With the above form for the $\{|p\,\rangle\}$-space representation of $|\psi(0)\,\rangle$, the calculation of $\langle P \rangle_{t=0}$ and $\langle (\Delta P)^2 \rangle_{t=0}$ are calculationally equivalent to what we already did for $\langle X \rangle_{t=0}$ and $\langle (\Delta X)^2 \rangle_{t=0}$, yielding

$$\langle P \rangle_{t=0} = p_0 \qquad \langle (\Delta P)^2 \rangle_{t=0} = \sigma_p^2 \tag{5.14}$$

The Free Particle (cont.)

We may now calculate $|\psi(t)\rangle$. Shankar does this only in the $\{|x\rangle\}$ basis, but we do it in the $\{|p\rangle\}$ basis too to illustrate how simple it is in the eigenbasis of H. The result is of course

$$\psi_p(p,t) = \langle p\,|\psi(t)\,\rangle = \left(\frac{1}{2\,\pi\,\sigma_p^2}\right)^{1/4} e^{-\frac{(p-p_0)^2}{4\,\sigma_p^2}}\, e^{-\frac{i}{\hbar}\,\frac{p^2}{2\,m}\,t} \tag{5.15}$$

That is, each $\{|p\rangle\}$ picks up a complex exponential factor for its time evolution. It is immediately clear that $\langle P\rangle$ and $\langle(\Delta P)^2\rangle$ are independent of time. Calculationally, this occurs because P, and $(\Delta P)^2$ simplify to multiplication by numbers when acting on $|p\rangle$ states and the time-evolution complex-exponential factor cancels out because the two expectation values involve $\langle\psi\,|$ and $|\psi\,\rangle$. Physically, this occurs because the P operator commutes with H; later, we shall derive a general result about conservation of expectation values of operators that commute with the Hamiltonian. Either way one looks at it, one has

$$\langle P\rangle_t = \langle P\rangle_{t=0} = p_0 \qquad \langle(\Delta P)^2\rangle_t = \langle(\Delta P)^2\rangle_{t=0} = \sigma_p^2 \tag{5.16}$$

The Free Particle (cont.)

Let's also calculate the $\{|x\rangle\}$ representation of $|\psi(t)\rangle$. Here, we can just use our propagator formula, Equation 5.6, which tells us

$$\psi_x(x,t) = \langle x\,|\psi(t)\,\rangle = \int_{-\infty}^{\infty} dx'\,[U(t)]_{xx'}\,\langle x'\,|\psi(0)\,\rangle$$

$$= \int_{-\infty}^{\infty} dx' \sqrt{\frac{m}{2\,\pi\,\hbar\,i\,t}}\, e^{\frac{i}{\hbar}\,\frac{m\,(x-x')^2}{2t}} \left(\frac{1}{2\,\pi\,\sigma_x^2}\right)^{1/4} e^{\frac{i}{\hbar}\,p_0\,x'}\, e^{-\frac{(x')^2}{4\,\sigma_x^2}}$$

$$= \left[\sqrt{2\,\pi\,\sigma_x^2}\left(1+\frac{i\,\hbar\,t}{2\,m\,\sigma_x^2}\right)\right]^{-1/2} \exp\left[-\frac{\left(x-\frac{p_0}{m}\,t\right)^2}{4\,\sigma_x^2\left(1+\frac{i\,\hbar\,t}{2\,m\,\sigma_x^2}\right)}\right]$$

$$\exp\left(\frac{i}{\hbar}\,p_0\,x\right)\exp\left(-\frac{i}{\hbar}\,\frac{p_0^2}{2\,m}\,t\right) \tag{5.17}$$

where we do the integral in the usual fashion, by completing the square and using the Gaussian definite integral.

The Free Particle (cont.)

The probability density in the $\{|x\rangle\}$ basis is

$$P(x) = |\langle x\,|\psi(t)\,\rangle|^2$$

$$= \left[2\,\pi\,\sigma_x^2\left(1+\left(\frac{\hbar\,t}{2\,m\,\sigma_x^2}\right)^2\right)\right]^{-1/2}\exp\left[-\frac{\left(x-\frac{p_0}{m}\,t\right)^2}{2\,\sigma_x^2\left(1+\left(\frac{\hbar\,t}{2\,m\,\sigma_x^2}\right)^2\right)}\right] \tag{5.18}$$

Because the probability density is symmetric about $x = \frac{p_0}{m}\,t$, it is easy to see that

$$\langle X\rangle_t = \frac{p_0}{m}\,t = \langle X\rangle_{t=0} + \frac{p_0}{m}\,t \tag{5.19}$$

i.e., the particle's effective position moves with speed p_0/m, which is what one expects for a free particle with initial momentum p_0 and mass m.

The Free Particle (cont.)

The variance of the position is given by the denominator of the argument of the Gaussian exponential (one could verify this by calculation of the necessary integral),

$$\langle (\Delta X)^2 \rangle_t = \sigma_x^2 \left[1 + \left(\frac{\hbar\, t}{2\, m\, \sigma_x^2} \right)^2 \right] = \langle (\Delta X)^2 \rangle_{t=0} \left[1 + \left(\frac{\hbar\, t}{2\, m\, \sigma_x^2} \right)^2 \right] \qquad (5.20)$$

The position uncertainty grows with time because of the initial momentum uncertainty of the particle – one can think of the $\{|p\rangle\}$ modes with $p > p_0$ as propagating faster than p_0/m and those with $p < p_0$ propagating more slowly, so the initial wavefunction spreads out over time. In the limit of large time ($t \gg 2\, m\, \sigma_x^2/\hbar$), the uncertainty $\sqrt{\langle (\Delta X)^2 \rangle_t}$ grows linearly with time. The "large time" condition can be rewritten in a more intuitive form:

$$t \gg t_0 = 2\, m\, \frac{\sigma_x^2}{\hbar} = m\, \frac{\sigma_x}{\sigma_p} = \frac{\sigma_x}{\sigma_v} \qquad (5.21)$$

where $\sigma_v = \sigma_p/m$ is the velocity uncertainty derived from the momentum uncertainty. So, t_0 is just the time needed for the state with typical velocity to move the width of the initial state. We should have expected this kind of condition because σ_x and $\hbar$ are the only physical quantities in the problem. Such simple formulae can frequently be used in quantum mechanics to get quick estimates of such physical phenomena; we shall make such use in the particle in a box problem.

The Free Particle (cont.)

Position-Momentum Uncertainty Relation

Before leaving the free particle, we note an interesting relationship that appeared along the way. Recall that, because the position and momentum operators do not commute, $[X, P] = i\hbar$, no state is an eigenstate of both. If there is no uncertainty in one quantity because the system is in an eigenstate of it, then the uncertainty in the other quantity is in fact infinite. For example, a perfect position eigenstate has a delta-function position-space representation, but it then, by the alternative representation of the delta function, Equation 3.146, we see that it is a linear combination of all position eigenstates with equal weight. The momentum uncertainty will be infinite. Conversely, if a state is a position eigenstate, then its position-space representation has equal modulus everywhere and thus the position uncertainty will be infinite.

The Free Particle (cont.)

When we considered the Gaussian wave packet, which is neither an eigenstate of X nor of P, we found that the $t = 0$ position and momentum uncertainties were

$$\langle (\Delta X)^2 \rangle_{t=0} = \sigma_x^2 \qquad \langle (\Delta P)^2 \rangle_{t=0} = \sigma_p^2 = \frac{\hbar^2}{4\,\sigma_x^2} \tag{5.22}$$

Hence, at $t = 0$, we have the uncertainty relation

$$\sqrt{\langle (\Delta X)^2 \rangle_{t=0}}\sqrt{\langle (\Delta P)^2 \rangle_{t=0}} = \frac{\hbar}{2} \tag{5.23}$$

We saw that, for $t > 0$, the position uncertainty grows while the momentum uncertainty is unchanged, so in general we have

$$\sqrt{\langle (\Delta X)^2 \rangle}\sqrt{\langle (\Delta P)^2 \rangle} \geq \frac{\hbar}{2} \tag{5.24}$$

We will later make a general proof of this uncertainty relationship between noncommuting observables.

The Hamiltonian

A "box" consists of a region of vanishing potential energy surrounded by a region of infinite potential energy:

$$V(x) = \lim_{V_0 \to \infty} \begin{cases} 0 & |x| \leq \frac{L}{2} \\ V_0 & |x| > \frac{L}{2} \end{cases} \tag{5.25}$$

It is necessarily to include the limiting procedure so that we can make mathematical sense of the infinite value of the potential when we write the Hamiltonian. Classically, such a potential completely confines a particle to the region $|x| \leq L/2$. We shall find a similar result in quantum mechanics, though we need a bit more care in proving it.

The classical Hamiltonian is

$$\mathcal{H}(x, p) = \frac{p^2}{2\,m} + V(x) \tag{5.26}$$

The Particle in a Box (cont.)

Postulate 2 tells us that the quantum Hamiltonian operator is

$$H(X, P) = \frac{P^2}{2\,m} + V(X) \tag{5.27}$$

Next, we want to obtain an eigenvalue-eigenvector equation for H. For the free particle, when $V(X)$ was not present, it was obvious we should work in the $\{|p\,\rangle\}$ basis because H was diagonal there, and then it was obvious how P acted in that basis and we could write down the eigenvalues and eigenvectors of H trivially. We cannot do that here because $V(X)$ and hence H is not diagonal in the $\{|p\,\rangle\}$ basis. Moreover, regardless of basis, we are faced with the problem of how to interpret $V(X)$. Our usual power-series interpretation fails because the expansion is simply not defined for such a function – its value and derivatives all become infinite for $|x| \geq L/2$.

Shankar glosses over this issue and jumps to the final differential equation; thereby ignoring the confusing part of the problem! We belabor it to make sure it is clear how to get to the differential equation from H and the postulates. The only sensible way we have to deal with the above is to write down matrix elements of H in the $\{|x\,\rangle\}$ basis because our Postulate 2 tells us explicitly what the matrix elements of X are in this basis. Doing that, we have

$$\langle x\,|H(X, P)|x\,'\,\rangle = \langle x\,|\frac{P^2}{2\,m}\,|x\,'\,\rangle + \langle x\,|V(X)\,|x\,'\,\rangle \tag{5.28}$$

The Particle in a Box (cont.)

Let's look at each term separately. For the first term, since it is quadratic in P, let's insert completeness to get the P's separated:

$$\begin{aligned}
\langle x \,|\frac{P^2}{2\,m}|x\,'\,\rangle &= \frac{1}{2\,m}\int_{-\infty}^{\infty} dx\,''\langle x\,|P\,|x\,''\,\rangle\langle x\,''\,|P|x\,'\,\rangle \\
&= -\frac{\hbar^2}{2\,m}\int_{-\infty}^{\infty} dx\,''\left[\frac{d}{dx}\,\delta(x-x\,'')\right]\left[\frac{d}{dx\,''}\,\delta(x\,''-x\,')\right] \\
&= -\frac{\hbar^2}{2\,m}\frac{d}{dx}\int_{-\infty}^{\infty} dx\,''\delta(x-x\,'')\left[\frac{d}{dx\,''}\,\delta(x\,''-x\,')\right] \\
&= -\frac{\hbar^2}{2\,m}\frac{d}{dx}\left[\frac{d}{dx}\,\delta(x-x\,')\right] \\
&= -\frac{\hbar^2}{2\,m}\,\delta(x-x\,')\,\frac{d^2}{d(x\,')^2}
\end{aligned} \tag{5.29}$$

where in last step we used Equation 3.127,

$$\frac{d^n}{dx^n}\delta(x-x\,') = \delta(x-x\,')\frac{d^n}{dx\,'^n}$$

For the second term, we can approach it using a limiting procedure. Suppose $V(X)$ were not so pathological; suppose it has a convergent power series expansion $V(X) = \sum_{k=0}^{\infty} V_k\, X^k$. Then, we would have

$$\begin{aligned}\langle x\,|V(X)\,|x'\,\rangle &= \sum_{k=0}^{\infty} V_k \langle x\,|\,X^k|x'\,\rangle = \sum_{k=0}^{\infty} V_k\,\left(x'\right)^k \langle x\,|x'\,\rangle \\ &= \sum_{k=0}^{\infty} V_k\,\left(x'\right)^k \delta(x-x') = \delta(x-x')\,V(x')\end{aligned}$$

where we have allowed X to act to the right on $|x'\,\rangle$. This is not a strict application of Postulate 2; if one wants to be really rigorous about it, one ought to insert completeness relations like we did for P^2. For example, for X^2 we would have

$$\begin{aligned}\langle x\,|X^2\,|x'\,\rangle &= \int_{-\infty}^{\infty} dx''\langle x\,|X|x''\,\rangle\langle x''\,|X\,|x'\,\rangle = \int_{-\infty}^{\infty} dx''\,x\,\delta(x-x'')\,x''\,\delta(x''-x') \\ &= x^2\delta(x-x') = (x')^2\delta(x-x')\end{aligned}$$

For X^k, we have to insert $k-1$ completeness relations and do $k-1$ integrals. The result will be of the same form.

The Particle in a Box (cont.)

The key point in the above is that we have figured out how to convert the operator function $V(X)$ into a simple numerical function $V(x)$ when $V(X)$ can be expanded as a power series. To apply this to our non-analytic $V(X)$, we could come up with an analytic approximation that converges to the non-analytic one as we take some limit. (One could use a sum of tan^{-1} or tanh functions, for example.) The point is that if we used the expansion and then took the limit, we would obtain a result identical to the above. So we write

$$\langle x \,|V(X)\,|x\,' \rangle = \delta(x - x\,')\, V(x\,') \tag{5.30}$$

With the above results, we have that the matrix elements of H are given by:

$$\langle x \,|H\,|x\,' \rangle = \delta(x - x\,') \left[-\frac{\hbar^2}{2\,m} \frac{d^2}{d(x\,')^2} + V(x\,') \right] \tag{5.31}$$

The Particle in a Box (cont.)

Thus, for an arbitrary state $|f\rangle$, we have that (using completeness as usual)

$$\begin{aligned}
\langle x|H|f\rangle &= \int_{-\infty}^{\infty} dx'\langle x|H|x'\rangle\langle x'|f\rangle \\
&= \int_{-\infty}^{\infty} dx'\delta(x-x')\left[-\frac{\hbar^2}{2\,m}\frac{d^2}{d(x')^2}+V(x')\right]f(x') \\
&= \int_{-\infty}^{\infty} dx'\delta(x-x')\left[-\frac{\hbar^2}{2\,m}\frac{d^2 f(x')}{d(x')^2}+V(x')\,f(x')\right] \\
&= -\frac{\hbar^2}{2\,m}\frac{d^2 f(x)}{dx^2}+V(x)\,f(x) \qquad (5.32)
\end{aligned}$$