Hilbert Spaces in Quantum Mechanics

MA 466
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The Classical Particle in a Box

Consider a particle of mass m constrained to move along the x axis under the influence of some potential function $V(x,t)$, where t is of course time. The force on the particle at any time is $-\frac{\partial V}{\partial x}(x,t)$. From Newton's second law $F = ma$ the classical model for the particle's motion is

$$m\ddot{x}(t) + \frac{\partial V}{\partial x}(x(t),t) = 0 \tag{1}$$

where $x = x(t)$ is the position of the particle at any time. With appropriate initial conditions (position, velocity) we can solve the second order DE (1) to find the particle's position at any later time.

It's worth noting that the total energy $E(t)$ of the particle at any time, kinetic plus potential, is given by

$$E(t) = \frac{1}{2}m\dot{x}^2(t) + V(x(t),t) \tag{2}$$

It's easy to check that if equation (1) holds and V is independent of t then $\frac{dE}{dt} = 0$, so the total energy is conserved.

The Quantum View

In quantum mechanics the particle's physical state is governed by a *wave function* $\psi(x,t)$. The function $\psi(x,t)$ is complex-valued, and one interpretation of ψ is as a probability density. Specifically, if we measure the position of the particle at time t then the probability of finding the particle between $x = a$ and $x = b$ is given by

$$\int_a^b |\psi(x,t)|^2\,dx. \tag{3}$$

Of course this means that

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2\,dx = 1 \tag{4}$$

at all times.

The function $\psi(x,t)$ is a solution to Schrödinger's equation,

$$i\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=V\psi \tag{5}$$

where V is the potential function (real-valued). Of course the condition (4) forces

$$\lim_{x\to-\infty}\psi(x,t)=\lim_{x\to\infty}\psi(x,t)=0 \tag{6}$$

at all times t. The same holds true for the spatial derivatives of ψ.

Note that equation (5) is linear, so that any solution can be re-scaled by multiplying by an appropriate constant to satisfy equation (4) at any specific time. Moreover, once normalized for any given time, the solution will stay normalized for all later times, for

$$\begin{aligned}\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^2\,dx &= \frac{d}{dt}\int_{-\infty}^{\infty}\psi(x,t)\overline{\psi(x,t)}\,dx\\ &= \int_{-\infty}^{\infty}(\psi_t(x,t)\overline{\psi(x,t)}+\psi(x,t)\overline{\psi_t(x,t)})\,dx\\ &= \int_{-\infty}^{\infty}((\frac{ih}{2m}\psi_{xx}-\frac{i}{h}V\psi)\overline{\psi}+(-\frac{ih}{2m}\overline{\psi_{xx}}+\frac{i}{h}V\overline{\psi})\psi)\,dx\\ &= \frac{ih}{2m}\int_{-\infty}^{\infty}(\psi_{xx}\overline{\psi}-\overline{\psi_{xx}}\psi)\,dx \end{aligned}\tag{7}$$

where we've made use of equation (5) to substitute out ψ_t and $\overline{\psi_t}$ (and slipped the time derivative inside the integral, which is permitted if ψ_t exists and is reasonably well-behaved). If we now integrate by parts in x in each term in equation (7) and use equation (6) (to take a derivative off of ψ_{xx}, put it onto ψ) we obtain

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^2\,dx=\frac{ih}{2m}\int_{-\infty}^{\infty}(|\psi_x|^2-|\psi_x|^2)\,dx=0.$$

Once ψ has been normalized as in equation (4) for any time t, it will remain normalized.

Observables and Operators

If we measure the position of the particle at any time, we don't obtain a deterministic result. The position of the particle is a random variable with density function $|\psi|^2(x,t)$; if we imagine a large ensemble of independent particles all of which are in "identical" states (i.e., have the same wave function), position measurements on any given system will yield random values with density function $|\psi(x,t)|^2$. The expected value $< x >$ of the position measurement (if taken at time t) comes straight from standard probability theory and is given by

$$< x >= \int_{-\infty}^{\infty} x|\psi(x,t)|^2\,dx. \tag{8}$$

Of course if position is not deterministic then it isn't clear how velocity should be defined. Nevertheless, we can try to define velocity as the derivative of $< x >$ with respect to t; velocity itself then becomes a kind of random variable. From equation (8) we can compute

$$\begin{aligned} \frac{d < x >}{dt} &= \frac{d}{dt}\int_{-\infty}^{\infty} x|\psi(x,t)|^2\,dx \\ &= \frac{ih}{2m}\int_{-\infty}^{\infty} x(\psi_{xx}\overline{\psi} - \overline{\psi_{xx}}\psi)\,dx \end{aligned} \tag{9}$$

where equation (9) follows in almost exactly the same manner as equation (7)—there's just an extra "x" along for the ride under the integral. If we integrate each term by parts above, to take a derivative off of ψ_{xx} or $\overline{\psi_{xx}}$ and put the derivative onto $x\psi$ or $x\overline{\psi}$, we find (after some cancelation, and assuming that ψ and its derivatives vanish at infinity) that

$$\frac{d < x >}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} (\psi\overline{\psi_x} - \psi_x\overline{\psi})\,dx \tag{10}$$

Integrate the first term by parts again, to transfer the x derivative onto ψ to find that

$$\frac{d < x >}{dt} = -\frac{i\hbar}{m}\int_{-\infty}^{\infty} \overline{\psi}\psi_x\,dx. \tag{11}$$

Actually, it's more conventional to work with momentum $p = mv$, rather than velocity. In this case we might write $< p >= m\frac{d<x>}{dt}$ and obtain

$$< p >= -ih\int_{-\infty}^{\infty} \overline{\psi}\psi_x\,dx. \tag{12}$$

This is the expected value of the momentum of the particle.

Finally, though, let's write both of equations (8) (expected position) and (12) (expected momentum) in the more telling forms

$$< x > = \int_{-\infty}^{\infty} \overline{\psi} x \psi \, dx \tag{13}$$

$$< p > = \int_{-\infty}^{\infty} \overline{\psi} \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi \, dx \tag{14}$$

Given a function $\phi \in L^2(-\infty, \infty)$, let M denote the densely defined unbounded operator $M\phi = x\phi(x)$, and let D denote the densely defined unbounded operator $D\phi = \frac{\hbar}{i} \frac{d\phi}{dx}$. Equation (13) states that in order to compute $< x >$ at any time we should take the wave function ψ for the system, apply the operator M (in the x variable), then take the inner product of $M\psi$ with ψ. In short, equation (13) can be abbreviated

$$< x >=< M\psi, \psi > \tag{15}$$

in standard mathematical Hilbert space notation. The operator M is called the "position operator". In the same vein, equation (14) states that $< p >$ is computed by applying the "momentum operator" D to ψ, then taking an inner product with ψ. Thus

$$< p >=< D\psi, \psi > . \tag{16}$$

Actually, physicists prefer the so-called "bracket" notation, and would write $< x >=< \psi | M | \psi >$ or just $< x >=< \psi | x | \psi >$, and $< p >=< \psi | D | \psi >$ or $< p >=< \psi | \frac{\hbar}{i} \frac{\partial}{\partial x} | \psi >$.

Equations (15) and (16) illustrate one of the most important facets of quantum mechanics: classical physical quantities are replaced with operators (generally densely defined and unbounded) that operate on a system's wave function to produce expected values of the system's observables. Schrödinger's equation dictates the time evolution of the wave function for the system.

It's also worth noting that we can not only compute expected values, but also variances. For example, we can compute the second moment S_{xx} of the position random variable as

$$S_{xx} =< x^2 >= \int_{-\infty}^{\infty} x^2 |\psi(x,t)|^2 \, dx \tag{17}$$

which is really just the statement that $S_{xx} =< M^2\psi, \psi >$. Then the traditional variance of the position becomes $\sigma_x^2 = S_{xx} - < x >^2$. Similarly we can compute the second moment of the momentum as

$$S_{pp} =< p^2 >=< D^2\psi, \psi >= \int_{-\infty}^{\infty} \overline{\psi} \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi \, dx \tag{18}$$

from which we compute $\sigma_p^2 = S_{pp} - < p >^2$.

More generally, any physical quantity y associated to the system that can be constructed as a polynomial combination $y = Q(x, p)$ has expected value

$$< y >=< Q(M, D)\psi, \psi >= \int_{-\infty}^{\infty} \overline{\psi} Q(x, \frac{\hbar}{i}\frac{\partial}{\partial x})\psi \, dx. \tag{19}$$

For example, kinetic energy, which can be expressed as $\frac{1}{2m}p^2$, is associated with the operator $-\frac{1}{2m}\hbar^2\frac{\partial^2}{\partial x^2}$.

Finally, it's worth noting that an observable always assumes a real value. As such, for any observable y with corresponding operator Y we have $< y >= \overline{< y >}$, so that

$$< y >=< Y\psi, \psi >= \overline{< Y\psi, \psi >} =< \psi, Y\psi > .$$

That is, the operator Y must be Hermitian or self-adjoint. You can easily check that both M and D are self-adjoint.

An Example: The Infinite Square Well

Consider a particle of mass m in an "infinite square well", say on the interval $I = (0, 1)$. What this means is that the potential function $V(x, t)$ is defined to be zero for $x \in I$, and $V(x) = \infty$ for x outside of I. The interpretation of this is that outside I we have a zero chance of finding the particle (since it would have to have acquired infinite energy to get there), and so we require $\psi \equiv 0$ for x not in I. We'll talk about the boundary conditions in a moment.

We thus seek a solution to Schrödinger's equation on the interval $(0, 1)$. Separate variables as $\psi(x, t) = \alpha(t)\beta(x)$, plug into equation (5) with $V \equiv 0$, and separate to find

$$i\frac{\alpha_t}{\alpha} = -\frac{\hbar}{2m}\frac{\beta_{xx}}{\beta} = E$$

for some constant $E > 0$ (or else we have no hope of obtaining Dirichlet or Neumann boundary conditions). The solution for $\alpha(t)$ and $\beta(x)$ is

$$\begin{aligned} \alpha(t) &= C_1 e^{iEt} && (20) \\ \beta(x) &= C_2 \sin(qx) + C_3 \cos(qx) && (21) \end{aligned}$$

where C_1, C_2, C_3 are arbitrary constants and $q = \sqrt{2mE/\hbar}$ (so $E = \frac{\hbar q^2}{2m}$.)

Now for the boundary conditions: we'll use $\psi(0,t) = \psi(1,t) = 0$ at all times. You can derive that these are the "correct" boundary conditions by replacing the condition $V = \infty$ outside I by $V = A < \infty$ and examining the behavior of ψ at the boundaries as $A \to \infty$. I don't want to do that right now—it will distract from the main point!

And the main point is this: with zero Dirichlet boundary conditions we are forced to take $C_3 = 0$ in equation (21), with $q = k\pi$ for some integer k. This means that $E = \frac{\hbar k^2 \pi^2}{2m}$ and any separable solution to Schrödinger's equation is of the form

$$\psi_k(x,t) = e^{i\frac{\hbar k^2 \pi^2}{2m}t}\phi_k(x) \tag{22}$$

for some integer k, where $\phi_k(x) = \sqrt{2}\sin(k\pi x)$ (the $\sqrt{2}$ is so that $\|\phi_k\|_2 = 1$). The general solution is given by

$$\psi(x,t) = \sum_{k=1}^{\infty} c_k e^{i\frac{\hbar k^2 \pi^2}{2m}t}\phi_k(x) \tag{23}$$

where the c_k can be determined from the initial condition. In fact, if $\psi(x,0) = f(x)$ then we take

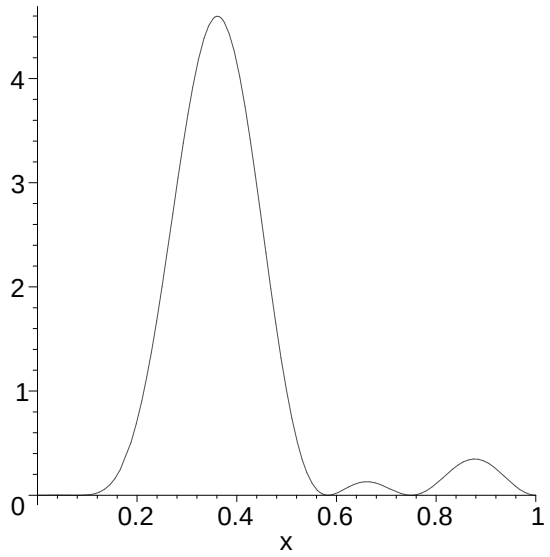
$$c_k = \int_0^1 f(x)\phi_k(x)\,dx. \tag{24}$$

The c_k might be real, but $\psi(x,t)$ will always be complex-valued due to the $e^{i\frac{\hbar k^2 \pi^2}{2m}t}$ factor. Note also that $e^{i\frac{\hbar k^2 \pi^2}{2m}t}$ is purely oscillatory and never decays away (in contrast to say, the heat equation).

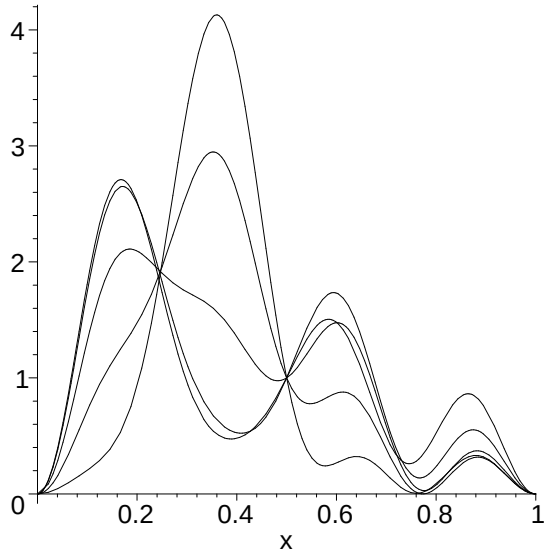
Let's compute the $< x >, \sigma_x, < p >$, and σ_p for such a particle. We'll take initial wave function $f(x) = \frac{\sqrt{2}}{2}\sin(\pi x) + \frac{1}{2}\sin(2\pi x) - \frac{1}{2}\sin(4\pi x)$ (note $|f|^2$ is normalized). This yields wave function

$$\psi(x,t) = \frac{\sqrt{2}}{2}e^{\frac{i\hbar\pi^2 t}{2m}}\sin(\pi x) + \frac{1}{2}e^{\frac{2i\hbar\pi^2 t}{m}}\sin(2\pi x) - \frac{1}{2}e^{\frac{8i\hbar\pi^2 t}{2m}}\sin(4\pi x). \tag{25}$$

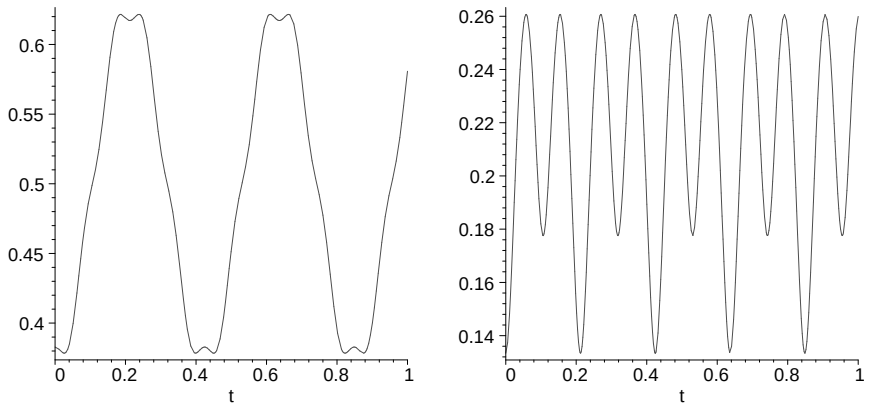
The square of the initial wave function amplitude at time $t = 0$ (with $\hbar = m = 1$, for simplicity) looks like



At times $t = 0.01, 0.02, 0.03, 0.04, 0.05$ the squared amplitude of the wave function looks like



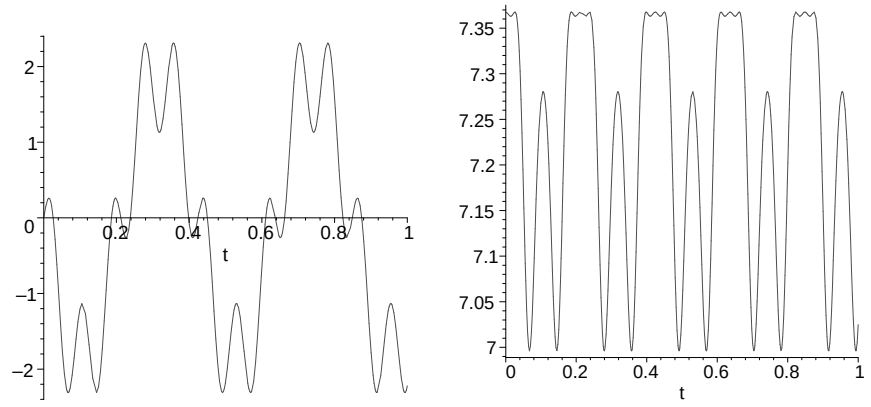
The figure on the left below shows that expected value $< x >$ as a function of time, while the figure on the right shows the standard deviation σ_x over time:



The actual formula for $< x >$ is

$$< x >= \frac{1}{2} - \frac{8\sqrt{2}}{9\pi^2} \cos\left(\frac{3\hbar\pi^2 t}{2m}\right) + \frac{16\sqrt{2}}{225\pi^2} \cos\left(\frac{15\hbar\pi^2 t}{2m}\right)$$

and isn't terribly enlightening. The formula for σ_x is messier. We can also compute and plot $< p >$ and σ_p over time, to obtain



The Uncertainty Principle

It's easy to see that $\sigma_x^2 \geq 0$ always, for $\sigma_x^2 =< M^2\psi, \psi > - < M\psi, \psi >^2$, so (using $\|\psi\| = 1$ and M self-adjoint)

$$\begin{aligned} \sigma_x^2 &= < M^2\psi, \psi > -(< M\psi, \psi >)^2 \\ &\geq < M\psi, M\psi > -\|M\psi\|^2 \\ &= 0 \end{aligned}$$

where I've used Cauchy-Schwarz in the form $< M\psi, \psi > \leq \|M\psi\|\|\psi\| = \|M\psi\|$. In fact, replace M by ANY self-adjoint operator Y to find $\sigma_y^2 \geq 0$. In particular, the same statement holds for momentum.

But in fact one can make a "joint" statement regarding the magnitude of σ_x and σ_p. Amazingly, this comes about from the innocuous fact that D and M do not commute. In fact, you can (and should) check that

$$DM - MD = \hbar I \tag{26}$$

where I is the identity operator. In what follows let us for simplicity just consider the case in which $< x >=< p >= 0$, which isn't too restrictive (we can always rescale position and velocity linearly so this is true, and it doesn't change the variances). In this case we have

$$\sigma_x^2 = \int_{-\infty}^{\infty} x^2 |\psi(x,t)|^2 \, dx = \|M\psi\|^2. \tag{27}$$

Also

$$\sigma_p^2 = -h^2 \int_{-\infty}^{\infty} \overline{\psi(x,t)} \frac{\partial^2 \psi}{\partial x^2} \, dx = h^2 \int_{-\infty}^{\infty} \frac{\overline{\partial \psi}}{\partial x} \frac{\partial \psi}{\partial x} \, dx = \|D\psi\|^2 \tag{28}$$

after an integration by parts. We then have

$$\begin{aligned} \hbar &= \hbar\|\psi\|^2 \\ &= \hbar| < \psi, \psi > | \\ &= | < (DM - MD\psi, \psi > | \\ &= | < DM\psi, \psi > - < MD\psi, \psi > | \\ &= | < M\psi, D\psi > - < D\psi, M\psi > | \\ &\leq 2\|M\psi\|\|D\psi\| \\ &= 2\sigma_x\sigma_p \end{aligned}$$

where I used the triangle inequality, Cauchy-Schwarz, and equations (27) and (28). Thus

$$\frac{\hbar}{2} \leq \sigma_x \sigma_p \tag{29}$$

which is the simplest version of the famous Heisenberg Uncertainty Principle. Note that the same computation works for ANY two observables with operators that do not commute. And if the operators a and b DO commute, the computations above will leave us empty handed with the uninteresting assertion $\sigma_a \sigma_b \geq 0$!

However, not every observable yields uncertain values when measured. Consider the same particle in a box as above, but with initial configuration $\psi(x,0) = \sqrt{2}\sin(2\pi x)$. It's straightforward to compute that

$$\begin{aligned} < x > &= 1/2 \\ \sigma_x^2 &= \frac{2\pi^2 - 3}{24\pi^2} \\ < p > &= 0 \\ \sigma_p^2 &= 4\pi^2\hbar^2. \end{aligned}$$

Nothing remarkable here—both position and momentum (as random variables) have non-zero variance (note also that $\sigma_p \sigma_x = \frac{\sqrt{12\pi^2 - 18}\hbar}{6} \approx 1.67\hbar > \hbar/2$, in accordance with the uncertainly principle. But if we use E to denote energy, with associated operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, we find

$$\begin{aligned} < E > &= \frac{2\pi^2\hbar^2}{m} \\ \sigma_E^2 &= 0. \end{aligned}$$

The energy of this system has NO variance—it will yield the same value each time!