Explanations of quantum animations

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I've produced a set of animations showing the time evolution of various wave functions in various potentials according to the Schrödinger equation. The point is to illustrate graphically some of the behaviors and points raised in lecture as well as to show some new and interesting quantum behavior beyond lecture (and beyond what you're responsible for this course).

The animations are MPEG4 format movie files. Most movies have arbitrary time and space units, so we are just studying the qualitative behavior here. I generated the movies using matlab. I include the source codes that generate these movies if you're interested and want to play with them (however, the comments are not great so ask me if you want to know what is going on). The matlab creates individual frames as JPEG images. I then use a free software (like MPEG Streamclip on Mac OS X) to take the JPEG files and string them into a MPEG4 movie. Another choice would have been to use the `getframe` and `movie` functions in matlab to show the animation inside matlab itself — but for some reason this wasn't working for me.

1 Barrier tunneling: tunneling.mp4

The idea here is to launch a particle at a barrier and to see it reflect and part of it be transmitted. To be able to talk intelligently about a particle coming from one side and going to the other side of the barrier, we must be dealing with a wave packet that is reasonably localized in space.

For this barrier tunneling animation, the potential is zero everywhere except in the region $-1 \leq x \leq 1$ where it has a height of 1. (You can see what I mean about arbitrary units). For purists, the units of distance are Bohr radii and of energy are Hartrees (1 Hartree=27.2 eV). In these units $\hbar^2/m = 1$ for an electron and we might as well set $\hbar = 1$ and $m = 1$ to make life easy.

We want to launch a wave packet with a pretty well defined energy. We will be launching it from the left (negative x) moving to the right so that it hits the barrier. The reflected wave will bounce back and move leftwards in the negative x region while the transmitted (tunneled) wave will be moving rightwards in the positive x region.

Since the potential is flat in the left region outside the well where we are starting the wave packet, its energy is purely kinetic: $E = p^2/(2m)$. So a very well-defined energy means a very well-defined momentum, but then the wave packet will have to be very wide by Heisenberg uncertainty. We must make a tradeoff. Here is a reasonable one: the initial starting wave is

$$\Psi(x,0) = C\exp\left(-\left[\frac{x-x_0}{\sigma}\right]^2\right) \times \Big[\cos(ik_0x) + i\sin(k_0x)\Big]\,.$$

This represents a (Gaussian) wave packet of width σ centered around x_0, with an average momentum of $\hbar k_0$ and moving rightwards for $k_0 > 0$, and C is a normalization constant. The animation was generated $\sigma = 20$, $k_0 = 1$, and $x_0 = -50$. Then this evolves according to Schrödinger's equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t)\,.$$

The simulation runs from $t = 0$ when the wave packet begins to move to the right until the time $t = L/(2\hbar k_0/m)$. The logic is that if the wave packet has an average momentum $\hbar k_0$, then its average speed is $\hbar k_0/m$ and thus this time is the time it takes it to go the distance $L/2$. Here the x-axis goes from $-L$ to L so the packet would move half the plotted range if there were no barrier.

With a choice of $k_0 = 1$, the average energy of this packet is $\hbar^2 k_0^2/(2m) = 1/2 = 0.5$. However, due to the uncertainty principle, the width σ gives some uncertainty in momentum and thus energy. For this case, the spread in energy is about 0.05 which is not that large (the energy spread is 10% the average value). For an energy of 0.5, a barrier height of 1.0, barrier width of 2, and with $\hbar^2/m = 1$, the penetration depth is

$$\eta = \frac{\hbar}{\sqrt{2m(U_{barrier} - E)}} = 1$$

and the tunneling probability is

$$P_{tunnel} = \exp(-2 \times \text{width}/\eta) = \exp(-4) \approx 1.8\%\,.$$

You can check that due to energy variation, the tunneling probability will also vary, but not by much: for the lower energy range of 0.45 it is 1.5% while for the higher energy range 0.55 it is 2.2%. So we expect about 2% tunneling probability.

What is plotted in the movie are the wave function $\Psi(x,t)$ and also the probability density $|\Psi(x,t)|^2$. Specifically, for each time t, we plot the spatial distribution $\Psi(x,t)$ — in other words snapshots. Since Ψ is complex, to honestly plot it one must plot both the real and imaginary parts (top two panels in blue and red, respectively). But you can just look at one or the other and the probability density to figure out what is happening; for our purposes, there is no real interest in Ψ having a real and imaginary part. Facts to note:

- As the movie rolls, the wave packet moves to the right as it should. It looks like it is rigidly being translated (not exactly correct, but the changes are very small and barely visible).
- When it gets to the region close to the origin, more interesting things happen. Part of the packet gets reflected by the barrier and part of it tunnels through. But while the packet is in the barrier region, there are lots of complicated looking oscillations as the wave interacts with the barrier.
- After a short time, most of the packet is reflected. You see a reflected packet depart leftwards away from the barrier.
- However, as the reflected packet goes its way, a small transmitted (tunneled) packet moves away to the right! This is the effect of quantum tunneling.
- After the packet leaves the region of the barrier, the remainder of the evolution looks pretty standard: two packets, each moving their own way and not interacting with each other.

- For those of you who want to think more deeply, if this wave packet represents an electron, we have wave function amplitude on *both* sides of the barrier and moving in opposite direction. And yet this represents a single electron: if you decide to measure to see which side the electron is on, you'll find it only on one side or the other. The outcome is probabilistic. But for any given measurement, if you see it on the left and reflected, then the amplitude on the right must vanish after the measurement. And vice versa. Quantum "particles" can become highly delocalized in a very unintuitive way: the "particle" has been split into to parts each moving in opposite directions and getting farther apart, and yet it is one coherent object when you measure it...

2 A free particle: free_particle_sig=20.mp4 & free_particle_sig=5.mp4

We didn't discuss this case in lecture, but it is some sense the simplest system. Namely, a particle that feels no potential anywhere so $U = 0$ everywhere. The classical analogue is a particle that feels no force. We'd expect it to just coast along at constant speed forever.

The first movie `free_particle_sig=20.mp4` has the same starting wave packet as the tunneling example above (but of course no barrier). As you can see, the packet just moves along at constant speed. If you look really carefully, you might notice some slight changes as it moves, but they're hard to see.

The second movie `free_particle_sig=5.mp4` has a starting wave packet that is four times narrower in space with $\sigma = 5$ instead but with the same momentum k_0. For this case, as the wave packet center moves to the right with the same speed as before, its width increases and its height decreases dramatically. (It "flattens".) This effect is due to what is called dispersion.

What is going on? A wave packet is spatially localized and thus must be made up of a superposition of different wavelengths. For the $\sigma = 20$ wave packet, Heisenberg uncertainty says $\sigma\Delta p \geq \hbar$ so we'd expect a spread in momentum of about $\Delta p = \hbar/20 = 0.05$ in our units. The average momentum is 1.0 so this is pretty small: the wider packet is made up of a narrow range of momenta or wavelengths (de Broglie). The narrower one has $\Delta p = 0.2$ which is now something like 20% of the average and is large: it has a much wider set of wavelengths or momenta composing it.

Now for an electron wave, were it to have a well-defined wavelength (i.e. be monochromatic or a pure sine wave), then its momentum $p = h/\lambda$ would be well-defined, its energy $E = p^2/(2m)$ too, and the Einstein relation $E = hf$ would give a frequency of $f = h/(2m\lambda^2)$. Notice that the wave speed $v = f\lambda = h/(2m\lambda)$ depends on λ! So different wavelengths move at different speeds.

This may seem bizarre: for light in vacuum $c = f\lambda$ is a constant. But the situation is actually quite general. Sound, water, and other material waves generally have wavelength dependent speeds of propagation. And even light, once it enters a material, has its speed reduced from c to c/n where n is the index of refraction and in general the index depends on lambda, so $n(\lambda)$. This wavelength dependence of the index is chromatic dispersion and makes a prism work.

For the electron wave packet, what this means is that we have a superposition of different wavelengths. As time goes on, the different components move at different speeds: the faster ones race ahead and the slower ones lag behind. So we expect the packet to get wider, and this is what you see. The narrower the initial packet, the wider the distributions of wavelengths composing it, and the worse the broadening effect since one has a wider range of velocities of its component waves.

3 Finite well: finite_well.mp4

We have a finite potential well. The potential inside the well is zero and outside is 1.0. The well's interior is $-50 \leq x << \leq 50$. We start a wave packet in the middle of the well moving to the right with $k_0 = 1.22$ and $\sigma = 20$. This gives it an energy of 0.75 (with energy spread 0.06) which is well below the barrier height: we don't expect this packet to be able to leave the potential well.

As you can see, indeed the wave packet hits the walls of the well (at $x = \pm 50$) and is completely reflected. But as it is undergoing reflection, there are some complex dynamics when it collides with the wall, and the wave function is clearly non-zero in the classically forbidden region beyond the wall of the well: we see the penetration depth effect.

4 Quantum harmonic oscillator: qho.mp4

A harmonic oscillator has potential $U(x) = kx^2/2$ which is smooth but always increasing. So a packet with any energy will eventually hit a turning point and get reflected back. From classical physics, you remember that the behavior is very regular and periodic with $x(t) = A\sin(\omega t + \phi)$ where ω is the angular frequency and given by $\omega = \sqrt{k/m}$. The periodic behavior has period $2\pi/\omega$ and is highly regular: after one period, the system returns to *exactly* where it was at the start.

Do any of these considerations carry over to the quantum case? The harmonic oscillator is a very special quantum system: its energy levels are extremely orderly and have uniform spacing. And the answer it mainly yes.

To see this and other physics, we study a harmonic oscillator with angular frequency $\omega = 1$ and choose units so $\hbar = 1$ too. We launch a Gaussian wave packet centered at the origin $x = 0$ with width $\sigma = 1$ and momentum rightwards $k_0 = 10$. Classically, the turning points would be at $x = \pm 10$ so we expect the wave packets to get reflected in these regions. As you run the movie, here are things to note:

- Indeed, the wave packet gets reflected back and forth. If you follow the center of the packet (where $|\Psi|^2$ is maximal) it traces the position a classical oscillator would have done! This is actually a general result in quantum mechanics that the center of the quantum probability distribution follows the classical trajectory $x(t)$ (or vice versa if you like). In this specific case, for a particle starting at the origin moving right and turning around at $x = 10$, the classical trajectory would be $x(t) = 10\sin(\omega t)$.

- When the wave packet is around the origin $x = 0$, it oscillates most rapidly while when it approaches the turning points it oscillates much less rapidly. This is simply because its kinetic energy decreases as it moves towards the turning points. Less kinetic energy means smaller momentum, and smaller momentum means longer wavelength from $\lambda = h/p$. So we are just seeing de Broglie in disguise.

- You'll notice that at first the wave packet widens so you think there may be irreversible dispersion like the free particle, but then after it reflects the squeezes back down again!

- Most impressively, after a full period $2\pi/\omega$ the wave packet is back where it started and has the same overall look. In fact, it is exactly the same wave packet in every detail. The harmonic oscillator, classical or quantum, has only a single frequency of behavior and so if you wait one period, it always comes back to its initial state exactly (classical or quantum). This is a consequence of the energy levels of the quantum oscillator being evenly spaced by always the same number $\hbar\omega$.

5 Infinite well: infinite_well.mp4

What could be simpler than the infinite well, you ask? Why did we leave this for the end? Well, it is simple but its behavior in terms of wave packets is much more complex than the nice harmonic oscillator.

To illustrate, we have a infinite well of width L=1. So the wave function is non-zero only for $0 < x < L$ and this is the only region we bother to show. A wave packet is launched from the center of the well ($x = 0.5$) moving to the right with momentum $k_0 = 50$ and width $\sigma = 0.15$. (The number are different than above because the size of the well is much smaller here.)

Classically, we expect this particle to bounce back and forth with fixed speed $\hbar k_0/m$: nothing could be simpler. But for the quantum version, because the energy levels are not evenly spaced, we get dispersive behavior and the packet widens as it moves. In a short time and after a few bounces of the wall, the whole thing looks like a gigantic mess because the packet gets as wide as the well itself and different parts reflect off the walls at different times and interfere with each other.

But be patient and keep watching! Weird things seem afoot as sometimes the waves seems to focus up. In fact, if you want until around 0.500 units of time, things will sharpen up: the big mess narrows down to a packet now moving leftwards from the center. Then things get messy again for a while, until at the end at 1.000 units of time the wave packet is completely and exactly restored to its original shape and form.

What is going on? The energy levels of the infinite well are $E_n = n^2 \cdot E_1$ where $E_1 = h^2/(8mL^2)$ is the ground-state energy of the well of size L. Thus the frequency of each is $f_n = E_n/h = n^2 f_1$. Since n is an integer, so is n^2 and thus all the frequencies of the different energy levels are integer multiples of the basic frequency of the lowest mode f_1. So as the system progresses, we have all sorts of different frequencies interfering — this makes for the mess. But since they have a very specific kind of relation, they do have a common period. Namely, one period of the lowest frequency $T_1 = 1/f_1$ is also a period for all the other modes.

Thus after a time $T_1 = 1/f_1 = h/E_1$ everything should be back in sync. This is an example of recurrence. For orderly systems with well-behaved energy levels, one will see the system return back to where it started after some fixed time. However, if the potential is not so nice (not harmonic or an infinite well) and energy levels have arbitrary relations to each other, we don't expect to see any recurrence at all since there is no shared period.

As a final note, the classical recurrence time (the time for two bounces to bring us where we started) is *not* the same as the quantum one. A classical particle of energy E in an infinite well has speed $v = \sqrt{2E/m}$ and, for a well of size L, it will perform two bounces (off left and right ends) in a time $T_{cl} = 2L/v = L\sqrt{2m/E}$. But the quantum version has only specific energies so it is hard to compare. So you might say let's plug the quantum energy into the classical formula. If you plug in $E = E_1 = h^2/(8mL^2)$ into the classical formula, what you get after minor algebra is $T_{cl} = 2h/E_1$ which is twice too long. This is due to the difference in phase and group velocity — an advanced topic you can read about on your own. In brief, the recurrence times are not the same and there are genuine differences between the quantum and classical infinite well.