Explanations of animations

This directory has a number of animations in MPEG4 format showing the time evolutions of various starting wave functions for the particle-in-a-box, the free particle, and the harmonic oscillator, as well as a scattering problem off a potential well. The idea is to see qualitatively what goes on.

For most of the movies have time and space units normalized by appropriate constants to make them dimensionless.

The programs generating the animations are matlab programs. I've included the source code in this directory. Feel free to read them, modify them, and make your own movies. Aside from matlab, you'll need some type of program to assemble all the digital files into a movie (e.g. Quicktime pro of a free movie software — I used MPEG Streamclip on a Mac OS X). The other choice is to use the `getframe` and `movie` functions in matlab to show the animation inside matlab itself.

1 Particle in a box

The box goes from $0 < x < a$. The x axis in these movies is thus x/a. Time units are in terms of the recurrence time $2h/E_1$. There are presently three animations.

(a) `particle_in_a_box_n=2.mp4`: here we start the system in the $n = 2$ stationary state at $t = 0$

$$\Psi(x,0) = \psi_2(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)$$

and let it evolve. The real and imaginary part do oscillatory behavior since

$$\Psi(x,t) = \Psi(x,0)\exp(-itE_2/\hbar)$$

is just a pure exponential. One main point is to see that the probability density $|\Psi(x,t)|^2$ doesn't change since this is a stationary state.

(b) `particle_in_a_box_halfofn=2.mp4` : This is the $n = 2$ state but the right half $x > a/2$ is zeroed off:

$$\Psi(x,0) = \begin{cases} \psi_2(x) & \text{if } 0 < x < a/2 \\ 0 & \text{else} \end{cases} .$$

This is <u>not</u> a stationary state. So the time-dependence is non-trivial. Roughly, the particle starts on the left side and should go to the right, then back left, etc. At least that is the classical expectation. It sort of happens, but the behavior in detail is clearly more complex.

(c) `particle_in_a_box_square_k=0.mp4` : here, $\Psi(x,0)$ is essentially a the square box function centered at the middle of the box that is zero for $|x - a/2| > \sigma$ and constant for $|x - a/2| < \sigma$,

$$\Psi(x,0) = \begin{cases} \sqrt{1/2\sigma} & \text{if } |x - a/2| < \sigma \\ 0 & \text{else} \end{cases} .$$

In this particular case $\sigma = a/10$.

(d) `particle_in_a_box_gauss_x=0_k=0.mp4` : here $\Psi(x,0)$ is a normalized Gaussian with width $\sigma = a/10$ centered at mix box,

$$\Psi(x,0) = C \exp\left(-\frac{(x-a/2)^2}{\sigma^2}\right) .$$

(e) `particle_in_a_box_gauss_k=50.mp4` : here $\Psi(x,0)$ is the same as (b) except that we give the state a momentum boost, specifically of $p_0 = \hbar k_0 = \hbar \times 50/a$,

$$\Psi(x,0) = C \exp\left(-\frac{(x-a/2)^2}{\sigma^2} + ik_0 x\right) .$$

In all cases (b)-(e), we see that initially the wave function spreads ('"dispersion"). Also, once it hits the walls it bounces back. Then things look rather complicated and not so interesting until we hit a half-recurrnce at $t = h/E_1$ and then full recurrence at $t = 2h/E_1$. For case (e) with nonzero momentum, the state actually moves to the right initially and bounces off the wall (as it spreads) which is what we expect it to do.

A finite momentum means an oscillatory and complex-valued wave function, so note that real and imaginary part. In cases (b)-(d), we start with a real wave function, but quickly evolve into one that is complex. Cases (c) and (d) are very similar qualitatively as they are essentially the same type of initial state: something localized about the center of the box with zero average momentum, so they spread out evenly in both directions. Case (e) is a quantum version of a particle starting in the middle of the box and moving to the right: classically it would bounce off the walls, and quantum mechanically the waves do reflect off the walls albeit in a complicated way.

2 Simple harmonic oscillator

For simplicity, we have set $m = 1$ and $\omega = 1$ to make the numbers easy.

(a) `qsho_gauss_w=1_x=0_k=7.mp4` : Here we start with a Gaussian of with $\sigma = 1$ ("w" in the movies) which is centered at the origin and has momentum of $p_0 = \hbar k_0 = \hbar \times 7/\sigma$. Classically, this momentum would have the particle turn around at around $\xi = 7$ (ξ is the standard dimensionless coordinate for the harmonic oscillator $\xi = [\sqrt{m\omega/\hbar}]x$).

(b) `qsho_n=0_translated_x=7.mp4` : Here the starting wave function is the ground-state of the harmonic oscillator $\psi_0(\xi)$ but translated to $\xi = 7$, namely $\Psi(x, t = 0) = \psi_0(\xi - 7)$.

What we see is clearly oscillation: the center of the packet moves in a simple way back and forth. The center of the packet obeys the Ehrenfest principle and will track the classical motion as we can see. Classically, the recurrence time is $2\pi/\omega$ and this is almost the same in quantum mechanics except for the zero-point contribution. It is easy to show that for the quantum harmonic oscillator when we write the initial wave function in the eigenbasis

$$\Psi(x,0) = \sum_n c_n \psi_n(x)$$

then

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-itE_n/\hbar} = \sum_n c_n \psi_n(x) e^{-it\hbar\omega(n+1/2)/\hbar} = \exp(-i\omega t/2) \sum_n c_n \psi_n(x) e^{-itn\omega} \,.$$

Thus the zero point contribution flips the sign at $t = 2\pi/\omega$,

$$\Psi(x, t = 2\pi/\omega) = -\Psi(x,0).$$

So you'll see that at the end of the movie, Ψ is minus what it started as. However, an overall phase makes no physical difference in any observable so for "practical" purposes of measuring any expectation value, we have recurrence for the quantum problem as well.

Note how in both cases, the momentum decreases as x increases and vice versa: the momentum is the "wigglines" of the wave function easily seen in terms of the oscillations of the real and imaginary part.

Finally, in case (b), if you look carefully, you'll note that the real and imaginary part may be changing, but the probability density is unchanged in shape and merely translates rigidly along the axis with the center of the Gaussian packet obeying the Ehrenfest principle and thus moving on the classical trajectory. The fact that there is no dispersion or change of width (as opposed to (a)) is a special consequence of the harmonic oscillator and choosing the translated ground state. In addition, if you were to calculate the Fourier transform of Ψ to see its momentum representation $\phi(k,t)$, it would also be a Gaussian whose width is fixed and whose center moves along the classical path (for $p(t)$ of course)! Last but not least, the uncertainty principle is obeyed at the limit at all times: $\sigma_x \sigma_p = \hbar/2$.

These are general phenomena for this class of functions (b) which are called "coherent states": in a well-defined sense they are closest to the classical analogue of an oscillator that we can get. Their center moves along the classical trajectory, the probability density translates rigidly without deforming, and at all times the packet obeys the uncertainty principle as an equality and is thus the best one can do. Making coherent states in this case is easy: just start with $\psi_0(x)$ and translate it off equilibrium and "let go", much like pulling on a mass on a spring and letting go to make it start oscillating. One could also not translate $\psi_0(x)$ but instead give it momentum boost: that would be like launching the classical particle from $x = 0$ with a kick. More general states with both average position off equilibrium and initial momentum are also easy to make by combining the two.

3 Free particle

Here we simulate wave packets of particles along an essentially infinite axis with zero potential everywhere.

(a) `free_particle_square_x=0_k=0.mp4` and `free_particle_gauss_x=0_k=0.mp4` : these are the same square and Gaussian functions as in the particle-in-a-box (a) and (b). They are centered about x=0. The widths σ are written as "w" in the movie file titles and axis labels.

(b) `free_particle_gauss_x=0_k=10.mp4` and `free_particle_square_x=0_k=10.mp4` : these are the same functions above but given a momentum boost by multiplying them by $exp(ik_0x)$ with $k_0 = 10/\sigma$.

As the movies show, with some momentum in case (b), the wave packet moves to the right as it should. In both cases, we see dispersion at play as the packet gets broader as times goes on. For the Gaussian cases, the shape in fact remains Gaussian and the width grows; for the square case, the evolution is more complex with some initial (transient) oscillations and changes in height.

In the cases (b) where the packet is moving, the center of the probability distribution (i.e. center of the packet) moves with the group velocity $v_g = p_0/m = \hbar k_0/m$. The "ripples" or "wiggles" however move at the phase velocity $v_\phi = p_0/(2m) = v_g/2$. You can see this by carefully looking at the movies and tracking how the crests of the ripples move backwards with respect to the center of the packet as time goes on and the packet moves.

4 Scattering off a potential well

Here we start with Gaussian wave packets much like the free particle case above, but there is an attractive potential well a the origin for the packet to scatter off of. The well is approximately a square well: a flat negative potential $-\alpha/a$ inside a region $|x| < a/2$ and zero outside. The "strength" of the potential (area under it) is $-\alpha$.

For small a, this is the delta function potential. For the delta well, the transmission coefficient is $T = 1/(1 + E/|E_b|)$ where E_b is the energy of the single bound state; the reflection coefficient is $R = 1 - T$.

To make life easy, I am using units for these animations where $\hbar = 1$ and $m = 1$. Time is measured again in units of $m\sigma^2/h$ where σ is the width of the Gaussian.

(a) We start with $\alpha = 2$ and $a = 0.5$. This potential has a single bound state at $E_b \approx -1.1$. The wave function of the bound state looks very much like that of a delta function well.

We start with a Guassian wave packet centered away from the well of $\sigma = 10$ and $k_0 = 10/\sigma$: we choose to relate σ and k_0 in this way in order to get a wave packet with reasonably well determined energy: the number of oscillations in the width is $\sim \sigma/\lambda = k_0\sigma/2\pi \sim 2$ so the wavelength is reasonably well defined. More quantitatively, the starting packet has average energy $\langle E \rangle = 0.51$ (all kinetic) and energy spread $\sigma_E = 0.1$.

`potscatter_sig=10_alpha=2_a=0.5.mp4` is the corresponding movie for the dynamics. Since the packet energy is below the bound state energy, we expect mostly reflection, and this is what you see: after the packet hits the potential well, one part of the wave reflects and another transmits and these two packets travel away from the well. And most of the weight is in the reflected wave.

(b) We not increase the packet's energy: $\sigma = 4$ and $k_0 = 10/\sigma$. Here $\langle E \rangle = 3.2$ and $\sigma_E = 0.6$. The potential is the same as (a). The corresponding movie is `potscatter_sig=4_alpha=2_a=0.5.mp4` and you can see that since the energy is higher than E_b, we get mostly transmission.

(c) For a more extreme case of high energy for the same potential as (a), $\sigma = 2$ and $k_0 = 10/\sigma$ gives $\langle E \rangle = 12.6$ and $\sigma_E = 2.5$. The corresponding movie is `potscatter_sig=2_alpha=2_a=0.5.mp4` and you have to look really carefully at the real and imaginary parts to see the little reflected part.

(d) Of course, if we have wave packets which don't have very well determined energy, the scattering off the potential will be much more complicated and hard to interpret. For the same potential as in (a), we now start with a Gaussian with $\sigma = 1$ and $k_0 = 1$: here the number of oscillations in the width σ is very small so the wavelength is not well defined. We have $\langle E \rangle = 1.0$ and $\sigma_E = 1.2$ which is more than 100% variation in energy all the way from below to above $|E_b|$. As you can see from the movie `potscatter_sig=1_k0=1_alpha=2_a=0.5.mp4`, the dynamics is complicated and hard to figure out, and probably a simple picture of just a signle transmission and reflection coefficient is not helpful.

(e) In this final movie, we start with the low energy wave packet of part (a) with $\sigma = 10$ and $k_0 = 10/\sigma$ with $\langle E \rangle = 0.51$. However, we widen and strengthen the potential to get multiple bound states. With $\alpha = 11$ and $a = 10$, I now get five bound states at in the finite square well with energies -1.05, -0.91, -0.69, -0.42, -0.12. As the movie `potscatter_sig=10_alpha=11_a=10.mp4` shows, almost all of the wave packet actually gets transmitted so this is not what we'd expect from the delta function analogy.

What happens in detail is hard to see — but you'll notice the dynamics around the origin when the packet is around the origin is different from (a). Qualitatively, with a wider well, the wave can bounce back and forth in the well region (multiple reflection) and interfere with itself. Thus for some particular energies we might expect very high transmission of the multiply reflected waves interfere destructively on the reflection side. This is basically the Ramasauer-Townsend effect.