Homework 1 Solution

1. Read the postulates, and if there is any weird vocabulary, look it up in the Quantum Vocabulary handout. If it’s not shown there, demand in the next lecture that Prof. Gruebele add it!

Don't worry if the postulates don’t make crystal-clear sense yet: that’s why we are spending a whole semester on quantum mechanics!

Solution: Hope you read them! Who knows, Gruebele might do a pop quiz... just kidding!

2. Write down the classical Hamiltonian (kinetic plus potential energy) of a 3-D particle in a gravitational potential $V(z) = mgz$ that depends only on height $z$, not on $x$ and $y$. Does the kinetic energy in 3-D depend on $p_x$ and $p_y$? Now write down the same Hamiltonian ignoring any kinetic energy in the $x$ and $y$ directions, i.e. the particle is only allowed to drop straight down, not to be thrown sideways in the gravitational field. Does the Hamiltonian depend on any other fundamental observables besides $z$ and $p_z$?

Solution: For a 3D particle, the kinetic energy $K = \frac{1}{2} m v^2 = \frac{(mv)^2}{2m} = \frac{p^2}{2m} = \frac{1}{2m} \left( p_x^2 + p_y^2 + p_z^2 \right)$. Thus it depends on all three momenta. Therefore,

$$H = K + V = \frac{p^2}{2m} + mgz = \frac{1}{2m} \left( p_x^2 + p_y^2 + p_z^2 \right) + mgz$$

is the total energy (kinetic + potential).

Thus, the kinetic energy depends on $p_x$ and $p_y$ also, even though the potential energy depends only on $z$. For example, if you throw a rock of a balcony, it flies away from the balcony sideways at constant velocity, and also drops downward.
If motion is restricted to the z axis only, \( H = \frac{p_z^2}{2m} + mgz \). So, the Hamiltonian is a function of only two fundamental variables \( z \) and \( p_z \).

**Turn in 3. (Graded out of 0-5)** On an x-\( p_x \) plot (where x is now the vertical axis, not z), draw the trajectory of a marble that starts at \( x=0 \), is thrown straight up at \( t=0 \), then falls back into the hand at \( x=0 \) at \( t>0 \) later. I started the plot for you below. Think it through carefully before drawing: right after the throw starts, the particle is still at \( x=0 \) but it has positive \( p_x \) and flies upward; eventually it slows down and stops in mid-air (\( p_x = ? \) then); then it falls down and therefore has negative \( p_x \). If energy is conserved, what is \( p_x \) when it lands in your hand again and \( x=0 \) again?

**Solution**

At \( t=0 \) (start of throw), \( x=0 \) and \( p_x \) is positive (considering velocity to be positive as the motion is along positive z axis). At the topmost part, there is zero velocity. As the marble comes down to the initial \( x=0 \) position, at \( t=t>0 \), its velocity (and momentum) is negative. Considering energy-momentum conservation, the final momentum is equal in magnitude and opposite in sign to the initial momentum.
4. Draw the quantum particle on the x-p plot for the same problem as in 3, but taking into account what Gruebele said about \( \Delta x \) and \( \Delta p \neq 0 \), i.e. the quantum particle’s center of mass location is not a point on the x-p plot.

Solution

For the quantum particle, the ‘trajectory’ of the wavefunction will be similar, but keep in mind that position and momentum cannot be determined simultaneously! So, when we can determine \( x \) with accuracy, there’ll be a finite uncertainty in \( p \), and vice versa. The product of the two uncertainties, however, will remain constant (\( \Delta x \Delta p = \frac{\hbar}{2} \)).

In the picture below, you can see that the wavefunction \( \Psi(p) \) (as a function of momentum) starts at positive momentum, and goes to negative momentum. The wavefunction as a function of position (good old \( \Psi(x) \), the one you’re more familiar with) starts out near \( x=0 \) (not shown), moves up to more positive \( x \) (2 examples shown) until it finally stops and turns around and comes back down. The center of the wavefunctions \( \Psi(x) \) and \( \Psi(p) \) traces out a path that looks pretty similar to the classical trajectory.

Next week, the TAs will tell you all about ‘Fourier transforms’, and the following week Gruebele will show you how \( x \) and \( p \) are related by the Heisenberg principle, and how the ‘Fourier transform’ can be used to convert from \( \Psi(x) \) to \( \Psi(p) \). In physics, they love to use \( \Psi(p) \). In chemistry or Chem E applications, we usually just deal with \( \Psi(x) \).