

# Homework H1 Solution

Problem 1: . Read the postulates...

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

Problem 2:

For a 3D particle, the kinetic energy

$$K = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{p^2}{2m} = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2).$$

Thus it depends on all three momenta. Therefore,

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

is the total energy (kinetic + potential).

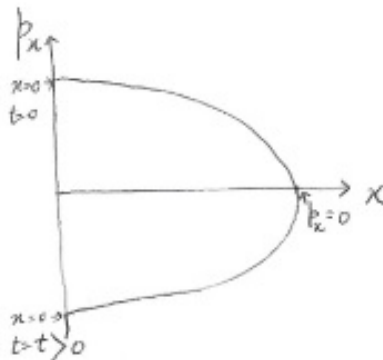
Thus, the kinetic energy depends on  $p_x$  and  $p_y$  also, even though the potential energy depends only on  $z$ . For example, if you throw a rock off a balcony, it flies away from the balcony sideways at constant velocity, and also drops downward.

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  $p_z$ .

## Problem 3 (turned in, out of 0 to 2 points):

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.

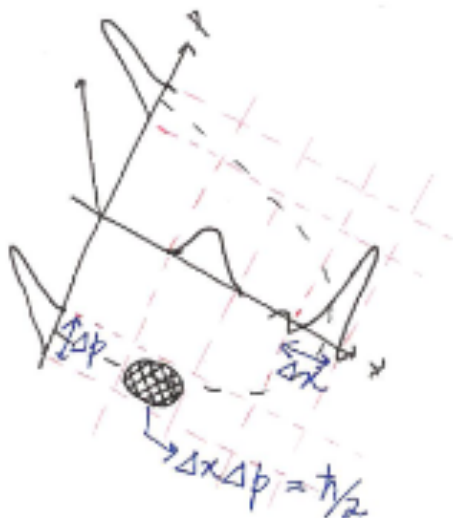
At  $t=0$  (start of throw),  $x=0$  and  $p_x$  is positive (considering velocity to be positive as the motion is along positive  $z$  axis). At the topmost part, there is zero velocity. As the marble comes down to the initial  $x=0$  position, at  $t=t>0$ , its velocity (and momentum) is negative. Considering energy-momentum conservation, the final momentum is equal in magnitude and opposite in sign to the initial momentum.



**Problem 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.

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  $p_x$ , and vice versa. The product of the two uncertainties, however, will remain constant ( $\Delta x \Delta p_x = \frac{\hbar}{2}$ ).

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  $\Psi(x)$ .