PHYS851 Quantum Mechanics I, Fall 2009
HOMEWORK ASSIGNMENT 6

1. [10 points] The quantum state of a free-particle of mass, M, at time t is a wave-packet of the form

$$\psi(x,t) = \frac{1}{\sqrt{\Gamma(5/4)\sigma_0}} e^{-\frac{(x-x_0)^4}{2\sigma_0^4} + ip_0x/\hbar},$$

We can safely predict that the width of the wave packet will grow in time. Clearly, the spreading velocity v_s must be determined by the initial conditions x_0, p_0, and σ_0, as well as the mass, M, and Planck's constant, $\hbar$, as there are no other parameters around to use.

(a) [2 pts] If there are no external forces acting on the particle, which parameters can we rule out based on symmetry arguments ?
The parameters x_0 and p_0 are depend on choice of coordinate system and inertial frame. The spread velocity of the wavefunction is not frame dependent. The basic equations for a free particle are invariant under boost and translation, therefore the spreading dynamics should not depend on frame-dependant parameters. Thus we conclude v_s does not depend on x_0 and p_0.

(b) [2 pts] Of the remaining parameters, how many unique ways are there to combine them to make an object with units of a velocity?
The remaining parameters are $\hbar$, M, and σ_0. Thus units of $\hbar$ are $\mathrm{kg\,m^2\,s^{-1}}$, thus any combination giving a velocity must depend only on $\hbar/M$, so that kg is cancelled. $\hbar/M$ has units $\mathrm{m^2\,s^{-1}}$, and the only parameter left is σ_0, which has units of length. Since we need a $\mathrm{s^{-1}}$ for velocity, the only possibility is

$$v = \frac{\hbar}{M\sigma_0}. \tag{1}$$

(c) [2 pts] Based on this result alone, give a units-based estimate for the velocity at which the wave-packet should spread.
The spread velocity must be

$$v_s \sim \frac{\hbar}{M\sigma_0}, \tag{2}$$

as there are no other possibilities.

(d) [2 pts] Again, by considering units alone, what energy scale, E_s, would you associate with a wave-packet of width σ_0?
From the width σ_0, and the constants $\hbar$ and M, the only energy we can form is

$$E_s = \frac{\hbar^2}{M\sigma_0^2}. \tag{3}$$

(e) [2 pts] We can assign a temperature to the wave-packet by setting $E_s = k_BT$. Solve this equation for σ_0 as a function of temperature, T. This is known as the thermal de Broglie wavelength, or the thermal coherence length, usually denoted as λ_{coh}. It gives the length-scale on which a particle at temperature T exhibits spatial coherence (quantum superposition).
If we set $k_BT = \hbar^2/(M\sigma_0^2)$, we find

$$\lambda_{coh} = \frac{\hbar}{\sqrt{Mk_BT}}. \tag{4}$$

This increases as the temperature decreases, which makes some kind of intuitive sense.

2. [10 points] The mass of a small virus is about 10^{-21}kg. What is the thermal coherence length of the virus at room temperature? What is it a liquid Helium temperature?

With $k_B \sim 10^{-23}$ and $\hbar \sim 10^{-34}$, we find that at room temperature, $T \sim 300\text{K}$, we find

$$\lambda_{coh}(300\text{K}) \sim \frac{10^{-34-(-21-23+2)/2}}{3} \sim 10^{-34+21-1} \sim 10^{-14}\text{m}. \tag{5}$$

At liquid Helium temperature, $T \sim 3\text{K}$, the temperature decreases by two orders of magnitude, so the coherence length increases by one order, giving

$$\lambda_{coh}(3\text{K}) \sim 10^{-13}\text{m} \tag{6}$$

Imagine a nano-scale double-slit apparatus consisting of a metal plate with two slits, each 1nm accross, with a center-to-center separation of 4nm. What coherence length is required in order to observe a double-slit interference pattern when passing many copies of the virus through the double-slit apparatus? Explain your reasoning.

In order to see interference, we need that each virus goes through both slits in a coherent superposition state, this requires that the coherence length be large enough to cover both slits. Thus we should have

$$\lambda_{coh} \sim 5\text{nm} \tag{7}$$

This is of the order 10^{-8}m, and would require a temperature decrease over liquid Helium temperature of 10 orders of magnitude, so we would need $T = 10^{-10}$K.

Assume that this coherence length can be obtained by velocity filtering. Based on what we have learned about wave-packet spreading, and assuming a longitudinal velocity of v_L, how far away from the apparatus would we need to put our detector in order to observe the interference fringes? Explain your reasoning

Assuming $\lambda_{coh} \geq 1$nm initially, after passing through a slit, the wavepacket of the virus will have collapsed to a width of $\sigma = 1$ nm. The packet will then start expanding at velocity

$$v_s = \frac{\hbar}{M\sigma} = 10^{-34+21+9} = 10^{-4}\text{m}\,\text{s}^{-1} \tag{8}$$

In order to see fringes, the screen must be far enough away that the right and left wavepackets have significant overlap. Thus a good criterion would be to set the width of each packet equal to the separation, $s = 4$nm, which implies a transit time of

$$t = \frac{s}{v_s} = \frac{4 \times 10^{-9}\text{m}}{10^{-4}\text{m}\,\text{s}^{-1}} = 4 \times 10^{-5}\text{s} = 40\,\mu\text{s} \tag{9}$$

the distance to the screen should therefore be $\geq v_L \cdot 4 \times 10^{-5}$s

3. [30 pts] Derive the equations of motion for $x(t) := \langle\psi(t)|X|\psi(t)\rangle$ and $p(t) := \langle\psi(t)|P|\psi(t)\rangle$, for a particle of mass M, in

   (a) free space, $V(X) = V_0$,

   (b) a uniform gravitational field, $V(X) = MgX$, where $g = 9.8\,\mathrm{m\,s^{-1}}$,

   (c) a harmonic oscillator potential $V(X) = \frac{1}{2}M\omega^2 X^2$.

   For each case, solve the equations, and give $x(t)$ and $p(t)$ in terms of the initial values $x(0)$ and $p(0)$.

   We learned in lecture that $\langle X\rangle$ and $\langle P\rangle$ obey the equations:

$$\frac{d}{dt}x(t) = \frac{p(t)}{M} \qquad (10)$$

$$\frac{d}{dt}p(t) = -\langle V'(X)\rangle \qquad (11)$$

   For (a), we have $V'(x) = \frac{\partial}{\partial x}V_0 = 0$, this gives:

$$\frac{d}{dt}x = \frac{p}{M} \qquad (12)$$

$$\frac{d}{dt}p = 0 \qquad (13)$$

   since we solved this equation as undergraduates, we know that the answer for initial conditions $x_0 = x(0)$ and $p_0 = p(0)$ is:

$$x(t) = x_0 + \frac{p_0}{M}t \qquad (14)$$

$$p(t) = p_0 \qquad (15)$$

   For case (b), we have $V'(x) = \frac{\partial}{\partial x}Mgx = Mg$, which gives

$$\frac{d}{dt}x = \frac{p}{M} \qquad (16)$$

$$\frac{d}{dt}p = -Mg \qquad (17)$$

   This has the solutions

$$x(t) = x_0 + \frac{p_0}{M}t - \frac{1}{2}g\,t^2 \qquad (18)$$

$$p(t) = p_0 - Mg\,t \qquad (19)$$

   For part (c) we have: $V'(x) = \frac{\partial}{\partial x}\frac{1}{2}M\omega^2x^2 = M\omega^2 x$, which gives

$$\frac{d}{dt}x = \frac{p}{M} \qquad (20)$$

$$\frac{d}{dt}p = -M\omega^2 x \qquad (21)$$

   The solutions to this well-known set of equations is

$$x(t) = x_0\cos(\omega t) + \frac{p_0}{M\omega}\sin(\omega t) \qquad (22)$$

$$p(t) = p_0\cos(\omega t) - M\omega x_0\sin(\omega t) \qquad (23)$$

4. [30 pts] For each of the three potentials in the above problem, derive a closed set of equations for

$$
\begin{aligned}
p^2(t) &:= \langle\psi(t)|P^2|\psi(t)\rangle, \\
xp(t) &:= \mathrm{Re}\langle\psi(t)|XP|\psi(t)\rangle = \frac{1}{2}\left[\langle\psi(t)|XP|\psi(t)\rangle + \langle\psi(t)|PX|\psi(t)\rangle\right], \\
x^2(t) &:= \langle\psi(t)|X^2|\psi(t)\rangle.
\end{aligned}
$$

For the initial conditions, $\langle X\rangle = 0$, $\langle P\rangle = 0$, $\langle X^2\rangle = \lambda_0^2/2$, $\langle XP\rangle = 0$ and $\langle P^2\rangle = \hbar^2/2\lambda_0^2$, solve the equations for the potentials in parts (a) and (b). (Hint: for (b) you will need to use your insert your results from the previous problem) For these initial conditions, we can interpret $x^2(t)$ as the square of the width of a wave-packet.

In general, we have

$$
\begin{aligned}
\frac{d}{dt}p^2 &= -\frac{i}{\hbar}\langle[P^2, H]\rangle \\
&= -\frac{i}{2M\hbar}\langle[P^2, P^2]\rangle - \frac{i}{\hbar}\langle[P^2, V(X)]\rangle \\
&= -\frac{i}{\hbar}\langle[P^2, V(X)]
\end{aligned}
\tag{24}
$$

$$
\begin{aligned}
\frac{d}{dt}x^2 &= -\frac{i}{\hbar}\langle[X^2, H]\rangle \\
&= -\frac{i}{2M\hbar}\langle[X^2, P^2]\rangle - \frac{i}{\hbar}\langle[X^2, V(X)]\rangle \\
&= -\frac{i}{2M\hbar}\langle[X^2, P^2]\rangle
\end{aligned}
\tag{25}
$$

and

$$
\begin{aligned}
\frac{d}{dt}xp &= -\frac{i}{2\hbar}\langle[XP + PX, H]\rangle \\
&= -\frac{i}{4M\hbar}\langle[XP + PX, P^2]\rangle - \frac{i}{2\hbar}\langle[XP + PX, V(X)]\rangle
\end{aligned}
\tag{26}
$$

Now

$$
\begin{aligned}
\left[P^2, V(X)\right] &= P^2V(X) - V(X)P^2 \\
&= P^2V(X) - PV(X)P + PV(X) - V(X)P^2 \\
&= P\left[P, V(X)\right] + \left[P, V(X)\right]P
\end{aligned}
\tag{27}
$$

using $[P, V(X)] = -i\hbar V'(X)$ then gives

$$
\left[P^2, V(X)\right] = -i\hbar\left(PV'(X) + V'(X)P\right) \tag{28}
$$

based on this result, we can immediately see that

$$
\left[X^2, P^2\right] = 2i\hbar\left(PX + XP\right) \tag{29}
$$

Then we find

$$
\begin{aligned}
\left[XP + PX, P^2\right] &= XP^3 - P^2XP + PXP^2 - P^3X \\
&= \left[X, P^2\right]P + P\left[X, P^2\right] \\
&= i\hbar\left(\frac{d}{dp}P^2\right)P + i\hbar P\left(\frac{d}{dp}P^2\right) \\
&= 4i\hbar P^2
\end{aligned}
\tag{30}
$$

and

$$\begin{aligned}[XP+PX,V(X)] &= XPV(X)-V(X)XP+PXV(X)-V(X)PX \\ &= X\left[P,V(X)\right]+\left[P,V(X)\right]X \\ &= -i\hbar XV'(X)-i\hbar V'(X)X \\ &= -2i\hbar XV'(X) \end{aligned} \tag{31}$$

putting this all together gives:

$$\frac{d}{dt}x^2 = \frac{2}{M}xp \tag{32}$$

$$\frac{d}{dt}xp = \frac{1}{M}p^2-\langle XV'(X)\rangle \tag{33}$$

$$\frac{d}{dt}p^2 = -\langle PV'(X)+V'(X)P\rangle \tag{34}$$

For $V(x)=V_0$ this gives

$$\frac{d}{dt}x^2 = \frac{2}{M}xp \tag{35}$$

$$\frac{d}{dt}xp = \frac{1}{M}p^2 \tag{36}$$

$$\frac{d}{dt}p^2 = 0 \tag{37}$$

This has the solution

$$p^2(t)=p^2(0)=\frac{\hbar^2}{2\lambda_0^2} \tag{38}$$

$$xp(t)=xp(0)+\frac{1}{M}p^2(0)t=\frac{\hbar^2}{2M\lambda_0^2}t \tag{39}$$

$$x^2(t)=x^2(0)+xp(0)t+\frac{1}{M^2}p^2(0)t^2=\frac{\lambda_0^2}{2}+\frac{\hbar^2}{2M^2\lambda_0^2}t^2 \tag{40}$$

For the gravitational potential, the equations are

$$\frac{d}{dt}x^2 = \frac{2}{M}xp \tag{41}$$

$$\frac{d}{dt}xp = \frac{1}{M}p^2-Mgx \tag{42}$$

$$\frac{d}{dt}p^2 = -2Mg\,p \tag{43}$$

from the previous problem, and with initial conditions $x_0=0$ and $p_0=0$, we know that

$$x(t) = -\frac{1}{2}g\,t^2 \tag{44}$$

$$p(t) = -Mg\,t \tag{45}$$

so this becomes

$$\frac{d}{dt}x^2 = \frac{2}{M}xp \tag{46}$$

$$\frac{d}{dt}xp = \frac{1}{M}p^2+\frac{1}{2}Mg^2\,t^2 \tag{47}$$

$$\frac{d}{dt}p^2 = 2M^2g^2\,t \tag{48}$$

Integrating these equations, starting with p^2, then gives

$$p^2(t) = p^2(0) + M^2 g^2 t^2 = \frac{\hbar^2}{2\lambda_0^2} + M^2 g^2\, t^2 \tag{49}$$

$$xp(t) = xp(0) + \frac{\hbar^2}{2M\lambda_0^2}t + \frac{1}{3}Mg^2\, t^3 + \frac{1}{6}Mg^2\, t^3 = \frac{\hbar^2}{2M\lambda_0^2}t + \frac{1}{2}Mg^2 t^3 \tag{50}$$

$$x^2(t) = x^2(0) + \frac{\hbar^2}{2M^2\lambda_0^2}t^2 + \frac{g^2}{4}t^4 = \frac{\lambda_0^2}{2} + \frac{\hbar^2}{2M^2\lambda_0^2}t^2 + \frac{g^2}{4}t^4 \tag{51}$$

(a) How does the free-space result compare to our previous result for the spreading of a Gaussian wave-packet?

For a gaussian of width σ centered at x_0, it is readily shown that $\langle X^2 \rangle = x_0^2 + \frac{\sigma^2}{2}$, thus we see that our results agree exactly with our previous calculation with the Gaussian wave-packet.

(b) Does the addition of a gravitational potential increase or decrease the spreading rate?

The addition of gravity appears to increase the rate of spreading. In fact, for long times, the width grows quadratically as t^2, rather than linearly in t.

(c) For potential (c), find the condition on λ_0 such that no spreading occurs. (You don't need to solve the equations, look for the condition so that all of the time-derivatives are zero)

The equations of motion for the case $V(x) = \frac{1}{2}M\omega^2 x^2$ are

$$\frac{d}{dt}x^2 = \frac{2}{M}xp \tag{52}$$

$$\frac{d}{dt}xp = \frac{1}{M}p^2 - M\omega^2 x^2 \tag{53}$$

$$\frac{d}{dt}p^2 = -2M\omega^2 xp \tag{54}$$

These equations have a steady state solution $x^2(t) = x^2(0)$, $xp(t) = xp(0)$, and $p^2(t) = p^2(0)$ for conditions

$$xp(0) = 0 \tag{55}$$

$$\frac{1}{M}p^2(0) = M\omega^2 x^2(0) \tag{56}$$

the first is already assumed to be true, the second requires

$$\frac{\hbar^2}{2M\lambda_0^2} = \frac{M\omega^2\lambda_0^2}{2} \tag{57}$$

solving for λ_0 gives

$$\lambda_0 = \sqrt{\frac{\hbar}{M\omega}} \tag{58}$$

which is interesting because this is the width of the ground-state wavefunction. Note that for the ground state, we would have $x(0) = 0$ and $p(0) = 0$, in which case it would makes sense that the width was constant, as we would be in a stationary state. But we have shown that the width is constant for all $x(0)$ and $p(0)$, if the initial width is given by (58). Since we know that $x(t)$ and $p(t)$ are in agreement with those of a classical particle, we see that wavepackets that oscillate like classical particles will not even spread if they have the right width. Such states are called 'coherent states', and they are thus the 'most classical' states for a quantum harmonic oscillator.

(d) **Extra credit:** Solve the equations for the potential in part (c), for the same initial conditions.

5. [5 pts] Consider the potential $V(X) = aX + bX^2 + cX^3$. Starting from the equation for $\langle X \rangle$, show that it is only possible to obtain a closed set of equations for the case $c = 0$.

The equation for $x(t)$ is, as usual,

$$\frac{d}{dt}x = \frac{1}{M}p \tag{59}$$

thus we need an equation for $p(t)$, which we know is going to be

$$\frac{d}{dt}p = -a + 2bx + 3cx^2 \tag{60}$$

thus we see that the set would have closed for $c = 0$, for $c \neq 0$, we now need the equation for x^2, which we know is

$$\frac{d}{dt}x^2 = \frac{2}{M}xp \tag{61}$$

and then the equation for $xp(t)$ is

$$\frac{d}{dt}xp = \frac{1}{M}p^2 - ax - 2bx^2 - 3cx^3 \tag{62}$$

thus in addition to p^2 which we would have expected, we now need an equation for x^3. The equation for p^2 is

$$\frac{d}{dt}p^2 = -2ap - 2bxp - 3c(px^2 + x^2p) \tag{63}$$

so there is even a new variable $px^2 + x^2p$. Clearly the set is never going to close, because at each step, the term proportional to c will generate terms of next-higher order.

6. [15 pts]For an incoming wave of energy E, find the wavefunction for all $x > 0$, for the potential

$$V(X) = \begin{cases} 0 & x > L \\ V_0 > 0 & 0 < x < L \\ \infty & x < 0 \end{cases}$$

Let us call the region $L < x$ 'Region I', and the region $0 < x < L$ 'Region II". The region $x < 0$ is forbidden. We then make the following ansatz:

$$\psi_1(x) = e^{-ikx} + re^{ikx}, \tag{64}$$

$$\psi_2(x) = ae^{iKx} + be^{-iKx} \tag{65}$$

where $k = \sqrt{2ME}/\hbar$ and $K = \sqrt{k^2 - k_0^2}$, where $k_0 = \sqrt{2M(E - V_0)}/\hbar$. The boundary condition at the edge of an infinite barrier is that the wavefunction must go to zero. Thus we have

$$\psi_2(0) = 0 \tag{66}$$

which means $b = -a$. We can thus change our ansatz to

$$\psi_2(x) = A\sin(Kx) \tag{67}$$

at $x = L$, we require

$$\psi_1(L) = \psi_2(L) \tag{68}$$

$$\psi_1'(L) = \psi_2'(L) \tag{69}$$

These boundary conditions lead to

$$e^{-ikL} + re^{ikL} = A\sin(KL) \tag{70}$$

$$ik(-e^{-ikL} + re^{ikL}) = AK\cos(KL) \tag{71}$$

solving the first for A gives

$$A = \frac{e^{-ikL} + re^{ikL}}{\sin(KL)} \tag{72}$$

plugging this into the second gives

$$ik(-e^{-ikL} + re^{ikL}) = (e^{-ikL} + re^{ikL})K\tan(KL) \tag{73}$$

solving for r then gives

$$r = e^{-2ikL}\frac{k - iK\tan(KL)}{k + iK\tan(KL)} \tag{74}$$

The wavefunction is thus given by

$$\psi(x) = 2e^{-ikL}\frac{[k\cos[k(x-L)] + K\tan(KL)\sin[k(x-L)]]\,u(x-L) + k\csc(KL)\sin(Kx)u(x)u(L-x)}{k + iK\tan(KL)} \tag{75}$$