Physics 139A Homework 2

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1 Problem 1

Classical mechanics is quantum mechanics - an alternative treatment of the QM of a particle on a line, based on the premise the position and momentum commute. The space of states is the space of square integrable functions of p and x, $\psi(p, x)$. We give up the idea that the Hamiltonian is the energy, because otherwise, with $H = E \equiv \frac{P^2}{2m} + V(x)$; we would have $i\hbar\frac{dx}{dt} = [H, x] = 0$. To get the right equations of motion for x and p, we instead postulate

$$H = -i\hbar\left[\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p}\right]$$

Verify that this gives the usual Newton equations for the time derivatives of x and p as a consequence of the Heisenberg equations. These equations lead to conservation of the energy E. Verify that also quantum mechanically $[H, E] = 0$. Write the Schrodinger equation for ψ and show that it implies that the probability density $\rho \equiv \psi * \psi$, satisfies the Liouville equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial E}{\partial p}\frac{\partial \rho}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial \rho}{\partial p}$$

Show that if $f(x, p)$ is a general function which is positive and has integral equal to 1, then

$$\rho(x, p, t) \equiv f(x(t), p(t))$$

is a solution of the Liouville equation. Here $x(t)$ and $p(t)$ are solutions of Newton's equations. If $x(0) = x$ and $p(0) = p$, then this is just a probability distribution for the position and momentum as a function of time that comes from deterministic evolution assuming f determined the probability distribution of unknown initial conditions. We can however make f a delta function without violating the equations, so all uncertainty here has to do with uncertainty in the initial state. Note that the phase of the wave function does not affect the expectation value of any function of x and p. As a quantum system, the model has other observables, the partial derivatives w.r.t x and p, which do not commute with these, but the Heisenberg equations do not relate x, p to these other variables. So, we can pretend they don't exist. The observations in this problem were made by Koopman in 1935, but they are not widely known. Our conclusion is that classical mechanics is a special case of QM, in which we can choose to ignore the non-commuting variables, since there's a complete set of equations of motion for variables that commute with each other

1.1 Proof of Postulate 1

Postulate 1.1.

$$H = -i\hbar \left[\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p} \right]$$

Proof. Now we use the Heisenberg equation (commutator of the Hamiltonian and an operator) to get the correct time derivatives of x and p.

$$\begin{aligned}
[H,x] =& -i\hbar \left(\frac{\partial \frac{p^2}{2m} + V(x)}{\partial p}\frac{\partial}{\partial x} - \frac{\partial \frac{P^2}{2m} + V(x)}{\partial x}\frac{\partial}{\partial p} \right) x - x \left(\frac{\partial \frac{p^2}{2m} + V(x)}{\partial p}\frac{\partial}{\partial x} - \frac{\partial \frac{P^2}{2m} + V(x)}{\partial x}\frac{\partial}{\partial p} \right) \\
[H,x] =& -i\hbar \left(\frac{p}{m}\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p} \right) x + i\hbar x \left(\frac{p}{m}\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p} \right) \\
[H,x] =& -i\hbar \left(\frac{p}{m}\frac{\partial x}{\partial x} - V'(x)\underbrace{\frac{\partial x}{\partial p}}_{=0} \right) + \underbrace{i\hbar x \left(\frac{p}{m}\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p} \right)}_{=0} \\
[H,x] =& -i\hbar\frac{p}{m} = i\hbar\frac{dx}{dt}
\end{aligned}$$

Which is what we want for the commutation of H and x. Now let us do the same thing except for p.

$$\begin{aligned}
[H,p] =& -i\hbar \left(\frac{\partial \frac{p^2}{2m} + V(x)}{\partial p}\frac{\partial}{\partial x} - \frac{\partial \frac{P^2}{2m} + V(x)}{\partial x}\frac{\partial}{\partial p} \right) p + i\hbar p \left(\frac{\partial \frac{p^2}{2m} + V(x)}{\partial p}\frac{\partial}{\partial x} - \frac{\partial \frac{P^2}{2m} + V(x)}{\partial x}\frac{\partial}{\partial p} \right) \\
[H,p] =& -i\hbar \left(\frac{p}{m}\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p} \right) x + i\hbar x \left(\frac{p}{m}\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p} \right) \\
[H,p] =& -i\hbar \left(\frac{p}{m}\underbrace{\frac{\partial p}{\partial x}}_{=0} - V'(x)\frac{\partial p}{\partial p} \right) + \underbrace{i\hbar p \left(\frac{p}{m}\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial p} \right)}_{=0} \\
[H,p] =& i\hbar V'(x) = -i\hbar F(x) = -i\hbar\frac{dp}{dt}
\end{aligned}$$

Once again gives us the proper time derivative of momentum p.

1.2 Proof of Lemma

Lemma 1.2. $[H,E] = 0$

Proof.

$$\begin{aligned}
[H,E] =& -i\hbar \left(\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p} \right) E + i\hbar E \left(\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p} \right) \\
[H,E] =& -i\hbar \left(\frac{\partial E}{\partial p}\frac{\partial E}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial E}{\partial p} \right) + \underbrace{i\hbar E \left(\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p} \right)}_{=0} \\
[H,E] =& -i\hbar \left(\frac{\partial E}{\partial p}\frac{\partial E}{\partial x} - \frac{\partial E}{\partial p}\frac{\partial E}{\partial x} \right) \\
[H,E] =& 0
\end{aligned}$$

1.3 Solution to Liouville Equation

1.3.1 Writing Schrodinger equation

The Schrodinger equation is as follows

$$\hat{H}\psi = i\hbar\frac{\partial}{\partial t}\psi$$

However, the complex conjugate will also satisfy the Schrodinger equation

$$\hat{H}\psi^* = i\hbar\frac{\partial}{\partial t}\psi^*$$

Therefore if we use our new formulation of the Hamiltonian we can write the Schrodinger equation as

$$-i\hbar\left[\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p}\right]\psi = i\hbar\frac{\partial}{\partial t}\psi$$

and it is also true for the complex conjugate of the wavefunction

$$-i\hbar\left[\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p}\right]\psi^* = i\hbar\frac{\partial}{\partial t}\psi^*$$

Simplifying both of these we get

$$\begin{aligned} -i\hbar\left[\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p}\right]\psi &= i\hbar\frac{\partial}{\partial t}\psi \\ \left[\frac{\partial E}{\partial p}\frac{\partial \psi}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial \psi}{\partial p}\right] &= \frac{\partial \psi}{\partial t} \end{aligned} \qquad \begin{aligned} -i\hbar\left[\frac{\partial E}{\partial p}\frac{\partial}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial}{\partial p}\right]\psi^* &= i\hbar\frac{\partial}{\partial t}\psi^* \\ \left[\frac{\partial E}{\partial p}\frac{\partial \psi}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial \psi}{\partial p}\right] &= \frac{\partial \psi}{\partial t} \end{aligned}$$

So now we see that both satisfy this equation so we can multiply the left column by the complex conjugate of ψ (or equivalently the right column by ψ) to obtain

$$\left[\frac{\partial E}{\partial p}\frac{\partial \psi^*\psi}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial \psi^*\psi}{\partial p}\right] = \frac{\partial \psi^*\psi}{\partial t}$$

And if we define $\rho \equiv \psi^*\psi$ as the probability density we arrive at the Liouville equation

$$\left[\frac{\partial E}{\partial p}\frac{\partial \rho}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial \rho}{\partial p}\right] = \frac{\partial \rho}{\partial t}$$

Finally let us define $\rho(x, p, t) \equiv f(x(t), p(t))$ and we can show that this satisfies the Liouville equation.

$$\begin{aligned} \left[\frac{\partial E}{\partial p}\frac{\partial f(x(t), p(t))}{\partial x} - \frac{\partial E}{\partial x}\frac{\partial f(x(t), p(t))}{\partial p}\right] &= \frac{\partial f(x(t), p(t))}{\partial t} \\ \frac{p}{m}\frac{\partial f}{\partial x} - V'(x)\frac{\partial f}{\partial p} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} \\ \frac{p}{m}\frac{\partial f}{\partial x} - V'(x)\frac{\partial f}{\partial p} &= \frac{\partial f}{\partial x}v + \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} \\ v\frac{\partial f}{\partial x} - V'(x)\frac{\partial f}{\partial p} &= \frac{\partial f}{\partial x}v + \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} \\ -V'(x)\frac{\partial f}{\partial p} &= \frac{\partial f}{\partial p}\frac{\partial p}{\partial t} \\ -V'(x) &= \frac{\partial p}{\partial t} \end{aligned}$$

But we know

$$F = -\frac{\partial V}{\partial x} = \frac{\partial p}{\partial t}$$

or in words, the negative of the derivative of the potential function is the force and the time derivative of the momentum is also force so that the generic function $f(x(t), p(t))$ is a solution to Liouville equation.

2 Problem 2.1

Prove the following theorems:

(a) For normalizable solutions, the seperation constant E must be real.

(b) ψ can always be taken to be real (unlike Ψ, which is necessarily complex).

(c) If $V(x)$ is an even function [i.e., $V(-x) = V(x)$], then $\psi(x)$ can always be taken to be either even or odd.

2.1 Solution to problem 2.1 Part A

Theorem 2.1. *For normalizable solutions, the seperation constant E must be real.*

Proof. We will prove this by contradiction. First assume E is complex such that it can be written as $E = E + i\Gamma$. The time dependent wavefunction is then

$$\Psi(x,t) = \psi(x)e^{iE/\hbar t}$$

Now applying normalizing conditions (Eq. 1.20) we find that

$$\begin{aligned}
1 &= \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx \\
1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 |e^{iE/\hbar t}|^2 dx \\
1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 dx |e^{i/\hbar(E+i\Gamma)t}|^2 \\
1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 dx e^{i/\hbar(E+i\Gamma)t} e^{-i/\hbar(E-i\Gamma)t} \\
1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 dx e^{i/\hbar(iE-\Gamma)t} e^{1/\hbar(-iE-\Gamma)t} \\
1 &= \underbrace{\int_{-\infty}^{\infty} |\psi(x)|^2 dx}\, e^{1/\hbar(iE-\Gamma)t} e^{1/\hbar(-iE-\Gamma)t}
\end{aligned}$$

The underlined portion is the only position dependent function, which happens to normalized. Hence this integral is 1.

$$\begin{aligned}
1 =& e^{t/\hbar(iE-\Gamma)+t/\hbar(-iE-\Gamma)} \\
1 =& e^{t/\hbar(iE-\Gamma-iE-\Gamma)} \\
1 =& e^{-2t\Gamma/\hbar}
\end{aligned}$$

Here we see that the RHS is time dependent and the LHS is not (it is equal to 1 always). The time dependence is entirely due to the complex part of the separation constant E, so we have reached a contradiction. The only way this can be true is if $\Gamma = 0$.

2.2 Solution to problem 2.1 Part B

Theorem 2.2. *The time-independent wavefunction ψ can always be taken to be real (unlike Ψ, which is necessarily complex).*

Proof. Starting with the time-independent Schrodinger equation we see that

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi =& E\psi \\
\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + (E-V)\psi =& 0 \\
\frac{d^2}{dx^2}\psi + \frac{2m}{\hbar^2}(E-V)\psi =& 0
\end{aligned}$$

Also, note that if $\psi(x)$ is a solution then its complex conjugate is solution too.

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi^* + V\psi^* =& E\psi^* \\
\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi^* + (E-V)\psi^* =& 0 \\
\frac{d^2}{dx^2}\psi^* + \frac{2m}{\hbar^2}(E-V)\psi^* =& 0
\end{aligned}
$$

Now we can say a linear combination is also a solution. There are two types of linear combinations that would make any complex solution a real solution, namely,

$$\psi_{real} = \psi + \psi^* \qquad and \qquad \psi_{real} = i(\psi - \psi^*)$$

This shows that any solution can always be written as a real function

2.2.1 Example of Theorem

If $V(x)$ is just a constant function (or step/well function) then the solutions are of the same form of the harmonic oscillator differential equation with $k = \frac{\sqrt{2m(E-V)}}{\hbar}$. This means the only solutions that satisfy this equation are sine's and cosine's and complex exponential's. However, complex exponential solutions can be expanded in terms of an imaginary part (sine) and and a real part (cosine), using Euler's formula. So the solutions are

$$
\begin{aligned}
\psi_R(x) =& Acos(kx) \\
\psi_R(x) =& Bsin(kx) \\
\psi_R(x) =& Csin(kx) + Dcos(kx) \\
\psi_C(x) =& Fe^{ikx} = F(cos(kx) + isin(kx))
\end{aligned}
$$

But we can see that the complex solution can be written entirely as a real cosine and real sine (or a combination of both). The complex wavefunction $\psi_C(x)$ can be written as a linear combination of itself and its complex conjugate such as

$$\psi_R(x) = (\psi_C(x) + \psi_C^*(x)) = 2Fcos(kx) \qquad or \qquad \psi_R(x) = i(\psi_C - \psi_C(x)) = 2Fsin(kx)$$

Which are both real, therefore, we can write any complex solution as a real function.

2.3 Solution to problem 2.1 Part C

Theorem 2.3. *If $V(x)$ is an even function [i.e., $V(-x) = V(x)$], then $\psi(x)$ can always be taken to be either even or odd.*

Proof. Once again starting with the time-independent Schrodinger equation we see that

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) =& E\psi(x) \\
\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + (E-V(x))\psi(x) =& 0 \\
\frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}(E-V(x))\psi(x) =& 0
\end{aligned}
$$

Now, if we replace $V(x)$ with $V(-x)$ (and consequently $\psi(x)$ with $\psi(-x)$) by letting $x \to -x$ we get

$$\frac{d^2}{dx^2}\psi(-x) + \frac{2m}{\hbar^2}(E-V(-x))\psi(-x) = 0$$

If $\psi(-x) = -\psi(x)$ (odd) then we get

$$
\begin{aligned}
\frac{d^2}{dx^2}\psi(-x) + \frac{2m}{\hbar^2}(E-V(x))\psi(-x) =& 0 \\
-\frac{d^2}{dx^2}\psi(x) - \frac{2m}{\hbar^2}(E-V(x))\psi(x) =& 0 \\
\frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}(E-V(x))\psi(x) =& 0
\end{aligned}
$$

If $\psi(-x) = \psi(x)$ (even) then we get

$$\frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

These produce square integrable solutions. Since any two linear solutions can be added to form another solution we can just add or subtract the even and odd solutions and obtain a general solution. Therefore, by definition of odd and even we can write the solution as a linear combination like $\psi_{even}(x) \pm \psi_{odd}(-x)$.

3 Problem 2.2

Show that E must exceed the minimum value of $V(x)$, for every normalizable solution to the time-independent Schrodinger equation. What is the classical analog of this statement?

3.1 Solution to Problem 2.2 Part A

Beginning with the Schrodinger equation we find

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + V\psi &= E\psi \\ \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + (E - V)\psi &= 0 \\ \frac{d^2}{dx^2}\psi + \frac{2m}{\hbar^2}(E - V)\psi &= 0 \\ \frac{d^2}{dx^2}\psi + k^2\psi &= 0 \end{aligned}$$

Where we have made the substitution $k = \frac{\sqrt{2m(E-V)}}{\hbar}$. Now we can see that the solution is entirely dependent on the quantity $E - V$. We have two situations at hand. The first is if $E > V$ then we get the differential equation

$$\frac{d^2}{dx^2}\psi + k^2\psi = 0$$

Which has known, square integrable solutions. The second case is $E < V$, which gives us the differential equation

$$\frac{d^2}{dx^2}\psi - k^2\psi = 0 \longrightarrow \psi = Ae^{-kx} + Be^{kx}$$

Which have permitted solutions of non-complex exponentials ($\psi(x) = e^{\pm kx}$). However, these standard exponential solutions are not square integrable over all space because they blow up at either infinity or negative infinity, hence can never be normalized.

3.2 Solution to Problem 2.2 Part B

The classical analog is a particle undergoing simple harmonic motion about an unstable equilibrium, or a point of maximum potential energy. Which is obviously ridiculous.

4 Problem 2.5

A particle in the infinite square well has its initial wave function an even mixture of the the first two stationary states:

$$\Psi(x, 0) = A[\psi_1(x) + \psi_2(x)]$$

(a) Normalize $\Psi(x, 0)$.

(b) Find $\Psi(x, t)$ and $|\Psi(x, t)|^2$

(c) Compute $\langle x \rangle$. What is the angular frequency of the oscillation? What is the amplitude of the oscillation?

(d) Compute $\langle p \rangle$.

(e) If you measured the energy of thus particle, what values might you get, and what is the probability of getting each of them? Find the expectation value of H. How does it compare with E_1 and E_2?

4.1 Solution to Problem 2.5 part A

The normalization condition is just

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1$$
$$\int_{-\infty}^{\infty} A^2[\psi_1(x)+\psi_2(x)]^2 dx = 1$$
$$\int_{-\infty}^{\infty} A^2[\psi_1^2(x)+\psi_2^2(x)+2\psi_1(x)\psi_2(x)] dx = 1$$
$$A^2\left[\int_{-\infty}^{\infty}\psi_1^2(x)dx+\int_{-\infty}^{\infty}\psi_2^2(x)dx+\underbrace{\int_{-\infty}^{\infty}2\psi_1(x)\psi_2(x)dx}_{=0}\right] = 1$$

The underlined term is zero due to the orthogonality of wavefunctions in an infinite square well. Refer to page 33 of Griffiths for more details of orthogonality or Boas chapter 3 or 12.

$$A^2\left[\int_{-\infty}^{\infty}\psi_1^2(x)dx+\int_{-\infty}^{\infty}\psi_2^2(x)\right]dx = 1$$
$$\boxed{A^2\,[1+1] = 1 \longrightarrow A = \frac{1}{\sqrt{2}}}$$

4.2 Solution to Problem 2.5 part B

4.2.1 Finding $\Psi(x,t)$

The energy eigenvalues of the stationary states of the infinite square well are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

And we know that $E = \hbar\omega$ therfore ,

$$\omega_n = \frac{E_n}{\hbar} = \frac{n^2\pi^2\hbar}{2ma^2}$$

We know that for stationary states in the infinite square well the time dependence is given by $\phi(t) = e^{i\omega_n t}$ (found by separation of variables when solving the Schrodinger equation). Each stationary state has a different time dependence, or frequency ω_n. ence, the full time dependent solution as

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{a}}sin(k_1x)e^{i\omega_1 t}+\sqrt{\frac{2}{a}}sin(k_2x)e^{i\omega_2 t}\right) = \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\left(sin(\tfrac{\pi}{a}x)e^{i\frac{\pi^2\hbar}{2ma^2}t}+sin(\tfrac{3\pi}{a}x)e^{i\frac{4\pi^2\hbar}{2ma^2}t}\right)}$$

4.2.2 Finding $|\Psi(x,t)|^2$

This product is actually $|\Psi(x,t)|^2 = \Psi(x,t)\Psi^*(x,t)$. This does not effect the sines but do affect the complex exponentials. Hence, the sine terms can just be squared but the exponential terms will be complex conjugate times itself.

$$|\Psi(x,t)|^2 = |\frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\left(sin(k_1x)e^{i\omega_1 t}+sin(k_2x)e^{i\omega_2 t}\right)|^2$$
$$|\Psi(x,t)|^2 = \frac{1}{a}\left(sin^2(k_1x)e^{i\omega_1 t}e^{-i\omega_1 t}+sin^2(k_2x)e^{i\omega_2}e^{-i\omega_2 t}+sin(k_1x)sin(k_2x)e^{i\omega_1 t}e^{-i\omega_2 t}+sin(k_1x)sin(k_2x)e^{i\omega_2 t}e^{-i\omega_1 t}\right)$$
$$|\Psi(x,t)|^2 = \frac{1}{a}\left(sin^2(k_1x)+sin^2(k_2x)+sin(k_1x)sin(k_2x)\left(e^{i(\omega_2-\omega_1)t}+e^{-i(\omega_2-\omega_1)t}\right)\right)$$
$$|\Psi(x,t)|^2 = \frac{1}{a}\left(sin^2(k_1x)+sin^2(k_2x)+2sin(k_1x)sin(k_2x)cos((\omega_2-\omega_1)t)\right)$$
$$|\Psi(x,t)|^2 = \frac{1}{a}\left(sin^2(\tfrac{\pi}{a}x)+sin^2(\tfrac{2\pi}{a}x)+2sin(\tfrac{\pi}{a}x)sin(\tfrac{2\pi}{a}x)cos((\tfrac{4\pi^2\hbar}{2ma^2}-\tfrac{\pi^2\hbar}{2ma^2})t)\right)$$
$$\boxed{|\Psi(x,t)|^2 = \frac{1}{a}\left(sin^2(\tfrac{\pi}{a}x)+sin^2(\tfrac{2\pi}{a}x)+2sin(\tfrac{\pi}{a}x)sin(\tfrac{2\pi}{a}x)cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\right)}$$

4.3 Compute $\langle x \rangle$

$$
\begin{aligned}
\langle x\rangle &= \int_0^a \Psi^*(x,t)x\Psi(x,t)dx \\
\langle x\rangle &= \frac{1}{a}\int_0^a x|\Psi(x,t)|^2 dx \\
\langle x\rangle &= \frac{1}{a}\int_0^a x\left(sin^2(\tfrac{\pi}{a}x)+sin^2(\tfrac{2\pi}{a}x)+2sin(\tfrac{\pi}{a}x)sin(\tfrac{2\pi}{a}x)cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\right)dx \\
\langle x\rangle &= \frac{1}{a}\left(\int_0^a xsin^2(\tfrac{\pi}{a}x)dx+\int_0^a xsin^2(\tfrac{2\pi}{a}x)dx+2\int_0^a xsin(\tfrac{\pi}{a}x)sin(\tfrac{2\pi}{a}x)cos((\tfrac{3\pi^2\hbar}{2ma^2})t)dx\right) \\
\langle x\rangle &= \frac{1}{a}\left(\underbrace{\int_0^a xsin^2(\tfrac{\pi}{a}x)dx}_{=\frac{a^2}{4}}+\underbrace{\int_0^a xsin^2(\tfrac{2\pi}{a}x)dx}_{=\frac{a^2}{4}}+2cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\underbrace{\int_0^a xsin(\tfrac{\pi}{a}x)sin(\tfrac{2\pi}{a}x)dx}_{=-\frac{8a^2}{9\pi^2}}\right) \\
\langle x\rangle &= \frac{1}{a}\left(\frac{a^2}{4}+\frac{a^2}{4}-\frac{16a^2}{9\pi^2}cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\right) \\
\langle x\rangle &= \frac{1}{a}\left(\frac{a^2}{2}-\frac{16a^2}{9\pi^2}cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\right)
\end{aligned}
$$

$$
\boxed{\langle x\rangle = a\left(\frac{1}{2}-\frac{16}{9\pi^2}cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\right)}
$$

Now the amplitude of oscillation and frequency are,

$$
\boxed{Amplitude = \frac{16a}{9\pi^2} < \frac{a}{2} \qquad\qquad \omega = \frac{3\pi^2\hbar}{2ma^2}}
$$

4.4 Computing $\langle p \rangle$

According to equation 1.33 in Griffiths

$$
\langle p\rangle = m\frac{d\langle x\rangle}{dt}
$$

Therefore we will just take the time derivative of average position $\langle x\rangle$ to get the average momentum.

$$
\begin{aligned}
\langle p\rangle &= m\frac{d\langle x\rangle}{dt} \\
\langle p\rangle &= m\frac{d}{dt}a\left(\frac{1}{2}-\frac{16}{9\pi^2}cos((\tfrac{3\pi^2\hbar}{2ma^2})t)\right) \\
\langle p\rangle &= -m\frac{d}{dt}\frac{16a}{9\pi^2}cos((\tfrac{3\pi^2\hbar}{2ma^2})t) \\
\langle p\rangle &= m\frac{3\pi^2\hbar}{2ma^2}\frac{16a}{9\pi^2}sin((\tfrac{3\pi^2\hbar}{2ma^2})t)
\end{aligned}
$$

$$
\boxed{\langle p\rangle = \frac{8\hbar}{3a}sin((\tfrac{3\pi^2\hbar}{2ma^2})t)}
$$

4.5 Energy probabilities of a non-stationary state

Since the original wavefunction is comprised of two equally weighted stationary states, the probability of finding the particle in the $n = 1$ states is 0.5 and the probability of finding the particle in the $n = 2$ state is also 0.5. We can refer back to section 4.1 to see why this is true. When we were normalizing the function (which is comprised of two stationary state wavefunctions) we observed that

$$
A^2\left[\int_{-\infty}^{\infty}\psi_1^2(x)dx+\int_{-\infty}^{\infty}\psi_2^2(x)\right]dx = 1
$$

which both integrals gave us one (because they are orthonormal), hence both have equal probability. The energy values the particle could have are

$$\boxed{E_1 = \frac{\pi^2\hbar^2}{2ma^2} \qquad E_2 = \frac{2\pi^2\hbar^2}{ma^2}}$$

Given that there is equal probability of finding the particle in either state the expectation value of of the Hamiltonian is just

$$\boxed{\langle H\rangle = P(E_1)E_1 + P(E_2)E_2 = \frac{1}{2}\frac{\pi^2\hbar^2}{2ma^2} + \frac{1}{2}\frac{4\pi^2\hbar^2}{2ma^2} = \frac{5\pi^2\hbar^2}{4ma^2}}$$

5 Problem 2.11

(a) Compute $\langle x\rangle, \langle p\rangle, \langle x^2\rangle, \langle p^2\rangle$ for states ψ_0 and ψ_1 of the harmonic oscillator, by explicit integration.

(b) Check the uncertainty principle for these states.

(c) Compute $\langle H\rangle$ and $\langle H\rangle$ for these states. Is their sum what you would expect?

5.1 Solution to Problem 2.11 part A

First we will state the first to states of the harmonic oscillator

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} \qquad \psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-\frac{m\omega}{2\hbar}x^2}$$

To simplify our algebra we will introduce the variables

$$\xi \equiv \sqrt{m\omega/\hbar x} \qquad \alpha \equiv \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

where now are wavefunctions become

$$\psi_0(x) = \alpha e^{-\frac{\xi^2}{2}} \qquad \psi_1(x) = \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}}$$

with

$$x = \sqrt{\hbar/m\omega}\xi \qquad and \qquad dx = \sqrt{\hbar/m\omega}d\xi$$

5.1.1 Computing $\langle x\rangle$

First we will compute $\langle x\rangle$ for ψ_0

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \psi_0^* x\psi_0 dx \\
\langle x\rangle &= \int_{-\infty}^{\infty} \alpha e^{-\frac{\xi^2}{2}} x\alpha e^{-\frac{\xi^2}{2}} dx \\
\langle x\rangle &= \alpha^2\int_{-\infty}^{\infty} \sqrt{\hbar/m\omega}\xi e^{-\xi^2} d\xi \\
\langle x\rangle &= \alpha^2\int_{-\infty}^{\infty} \sqrt{\hbar/m\omega}\xi e^{-\xi^2} d\xi \\
&\boxed{\langle x\rangle = 0}
\end{aligned}$$

The last integral is zero because it is an odd function being integrated over a symmetric domain.

Now, let us compute $\langle x \rangle$ for ψ_1

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi_1^* x \psi_1 dx$$
$$\langle x \rangle = \int_{-\infty}^{\infty} \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} x \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} dx$$
$$\langle x \rangle = 2\alpha^2 \int_{-\infty}^{\infty} \xi^2 e^{-\frac{\xi^2}{2}} x e^{-\frac{\xi^2}{2}} dx$$
$$\langle x \rangle = 2\alpha^2 \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} \sqrt{\hbar/m\omega}\xi \sqrt{\hbar/m\omega} d\xi$$
$$\langle x \rangle = 2\alpha^2 \hbar/m\omega \int_{-\infty}^{\infty} \xi^3 e^{-\xi^2} d\xi$$
$$\boxed{\langle x \rangle = 0}$$

This integral is zero also because it too is also odd. This is because

$$\int_{-\infty}^{\infty} x^{2n+1} e^{-x^2} dx = 0 \qquad \forall\, n \,\epsilon\, \mathbb{Z}$$

5.2 Computing $\langle p \rangle$

First we will compute $\langle p \rangle$ for ψ_0

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi_0^* \hat{p} \psi_0 dx$$
$$\langle p \rangle = -\int_{-\infty}^{\infty} \psi_0^* i\hbar \frac{\partial}{\partial x} \psi_0 dx$$
$$\langle p \rangle = -\int_{-\infty}^{\infty} \alpha e^{-\frac{\xi^2}{2}} i\hbar \frac{\partial}{\partial x} \alpha e^{-\frac{\xi^2}{2}} dx$$
$$\langle p \rangle = -\alpha^2 \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} i\hbar \sqrt{\hbar/m\omega} x e^{-\frac{\xi^2}{2}} \sqrt{\hbar/m\omega} d\xi$$
$$\langle p \rangle = -\alpha^2 \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} i\hbar \xi e^{-\frac{\xi^2}{2}} \sqrt{\hbar/m\omega} d\xi$$
$$\langle p \rangle = -i\hbar\alpha^2 \sqrt{\hbar/m\omega} \int_{-\infty}^{\infty} \xi e^{-\xi^2} d\xi$$
$$\boxed{\langle p \rangle = 0}$$

By same argument as the previous two integrals, this integral is also zero. Now we will compute $\langle p \rangle$ for ψ_1

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi_1^* \hat{p} \psi_1 dx$$
$$\langle p \rangle = -\int_{-\infty}^{\infty} \psi_1^* i\hbar \frac{\partial}{\partial x} \psi_1 dx$$
$$\langle p \rangle = -\int_{-\infty}^{\infty} \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} i\hbar \sqrt{\frac{m\omega}{\hbar}} \frac{\partial}{\partial \xi} \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} dx$$
$$\langle p \rangle = -2i\hbar\alpha^2 \sqrt{\frac{m\omega}{\hbar}} \int_{-\infty}^{\infty} \xi e^{-\frac{\xi^2}{2}} (1-2\xi^2) e^{-\frac{\xi^2}{2}} \sqrt{\hbar/m\omega} d\xi$$
$$\langle p \rangle = -2i\hbar\alpha^2 \int_{-\infty}^{\infty} (\xi - 2\xi^3) e^{-\xi^2} d\xi$$
$$\langle p \rangle = -2i\hbar\alpha^2 \left[\int_{-\infty}^{\infty} \xi e^{-\xi^2} d\xi - 2\int_{-\infty}^{\infty} \xi^3 e^{-\xi^2} d\xi \right]$$
$$\boxed{\langle p \rangle = 0}$$

Both integrals are zero once again because they are odd functions and we are integrating over a symmetric domain.

5.3 Computing $\langle x^2 \rangle$

First we will compute $\langle x^2 \rangle$ for ψ_0. We will need to know two integrals though first. They were proven using differentiation under an integral sign in Homework assignment 1. They are

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} dx = \frac{\sqrt{\pi}}{2} \qquad \int_{-\infty}^{\infty} x^4 e^{-x^2} dx = \frac{3\sqrt{\pi}}{4}$$

Now let us compute $\langle x^2 \rangle$ for ψ_0

$$\begin{aligned}
\langle x^2 \rangle &= \int_{-\infty}^{\infty} \psi_0^* x^2 \psi_0 dx \\
\langle x^2 \rangle &= (\hbar/m\omega)^{3/2} \int_{-\infty}^{\infty} \alpha e^{-\frac{\xi^2}{2}} \xi^2 \alpha e^{-\frac{\xi^2}{2}} d\xi \\
\langle x^2 \rangle &= (\hbar/m\omega)^{3/2} \alpha^2 \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi \\
\langle x^2 \rangle &= (\hbar/m\omega)^{3/2} \alpha^2 \frac{\sqrt{\pi}}{2} \\
\langle x^2 \rangle &= (\hbar/m\omega)^{3/2} \sqrt{\frac{m\omega}{\pi\hbar}} \frac{\sqrt{\pi}}{2} \\
&\boxed{\langle x^2 \rangle = \frac{\hbar}{2m\omega}}
\end{aligned}$$

Now let us compute $\langle x^2 \rangle$ for ψ_1

$$\begin{aligned}
\langle x^2 \rangle &= \int_{-\infty}^{\infty} \psi_1^* x^2 \psi_1 dx \\
\langle x^2 \rangle &= (\hbar/m\omega)^{3/2} \int_{-\infty}^{\infty} \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} \xi^2 \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} d\xi \\
\langle x^2 \rangle &= 2(\hbar/m\omega)^{3/2} \alpha^2 \int_{-\infty}^{\infty} \xi^4 e^{-\xi^2} d\xi \\
\langle x^2 \rangle &= 2(\hbar/m\omega)^{3/2} \alpha^2 3 \frac{\sqrt{\pi}}{4} \\
\langle x^2 \rangle &= (\hbar/m\omega)^{3/2} \sqrt{\frac{m\omega}{\pi\hbar}} \frac{\sqrt{\pi}}{2} \\
&\boxed{\langle x^2 \rangle = \frac{3\hbar}{2m\omega}}
\end{aligned}$$

5.4 Computing $\langle p^2 \rangle$

We will need to know what some derivatives are before we continue.

$$\frac{\partial^2}{\partial x^2} x e^{-x^2} = 2x(x^2-3)e^{-x^2} \qquad \frac{\partial^2}{\partial x^2} e^{-x^2} = (x^2-1)e^{-x^2}$$

First we will compute $\langle p^2 \rangle$ for ψ_0

$$\begin{aligned}
\langle p^2 \rangle &= \int_{-\infty}^{\infty} \psi_1^* \hat{p}^2 \psi_1 dx \\
\langle p^2 \rangle &= (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} \alpha e^{-\frac{\xi^2}{2}} \hbar^2 \frac{\partial^2}{\partial \xi^2} \alpha e^{-\frac{\xi^2}{2}} d\xi \\
\langle p^2 \rangle &= -\alpha^2 (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} e^{-\frac{\xi^2}{2}} \hbar^2 \frac{\partial^2}{\partial \xi^2} e^{-\frac{\xi^2}{2}} d\xi \\
\langle p^2 \rangle &= -\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} \xi e^{-\frac{\xi^2}{2}} (\xi^2-1) e^{-\frac{\xi^2}{2}} d\xi \\
\langle p^2 \rangle &= -\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} (\xi^2-1) e^{-\xi^2} d\xi \\
\langle p^2 \rangle &= -\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \left[\int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi - \int_{-\infty}^{\infty} e^{-\xi^2} d\xi \right] \\
\langle p^2 \rangle &= -\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \left[\frac{\sqrt{\pi}}{2} - \sqrt{\pi} \right] \\
&\boxed{\langle p^2 \rangle = \frac{m\hbar\omega}{2}}
\end{aligned}$$

Now we will compute $\langle p^2 \rangle$ for ψ_1.

$$\begin{aligned}
\langle p^2 \rangle &= \int_{-\infty}^{\infty} \psi_1^* \hat{p}^2 \psi_1 dx \\
\langle p^2 \rangle &= (\hbar/m\omega)^2 \int_{-\infty}^{\infty} \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} \hbar^2 \frac{\partial^2}{\partial \xi^2} \alpha\sqrt{2}\xi e^{-\frac{\xi^2}{2}} d\xi \\
\langle p^2 \rangle &= -2\alpha^2 (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} \xi e^{-\frac{\xi^2}{2}} \hbar^2 \frac{\partial^2}{\partial \xi^2} \xi e^{-\frac{\xi^2}{2}} d\xi \\
\langle p^2 \rangle &= -2\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} \xi e^{-\frac{\xi^2}{2}} 2\xi(\xi^2-3) e^{-\frac{\xi^2}{2}} d\xi \\
\langle p^2 \rangle &= -2\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \int_{-\infty}^{\infty} 2(\xi^4-3\xi^2) e^{-\xi^2} d\xi \\
\langle p^2 \rangle &= -4\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \left[\int_{-\infty}^{\infty} \xi^4 e^{-\xi^2} d\xi - 3\int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi \right] \\
\langle p^2 \rangle &= -4\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \left[\frac{3\sqrt{\pi}}{4} - 3\frac{\sqrt{\pi}}{2} \right] \\
\langle p^2 \rangle &= -4\hbar^2 \alpha^2 (\hbar/m\omega)^{1/2} \left[\frac{3\sqrt{\pi}}{4} - 3\frac{\sqrt{\pi}}{2} \right] \\
&\boxed{\langle p^2 \rangle = \frac{3m\hbar\omega}{2}}
\end{aligned}$$

5.5 Checking the uncertainty principle

First we must compute the standard deviations of the momentum and position for both the ground state and the first excited state. The standard deviation is just

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \qquad \sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

But for both cases $\langle p\rangle = 0$ and $\langle x\rangle = 0$ so we get that the standard deviations are just

$$\sigma_x = \sqrt{\langle x^2\rangle} \qquad\qquad \sigma_p = \sqrt{\langle p^2\rangle}$$

5.5.1 Ground State Uncertainty

For the ground state we have

$$\sigma_x = \sqrt{\langle x^2\rangle} = \sqrt{\frac{\hbar}{2m\omega}} \qquad\qquad \sigma_p = \sqrt{\langle p^2\rangle} = \sqrt{\frac{\hbar}{2m\omega}}$$

Now combining these two we get

$$\boxed{\sigma_x\sigma_p = \sqrt{\frac{\hbar}{2m\omega}}\sqrt{\frac{\hbar m\omega}{2}} = \frac{\hbar}{2} \quad \checkmark}$$

5.5.2 First Excited State Uncertainty

For the ground state we have

$$\sigma_x = \sqrt{\langle x^2\rangle} = \sqrt{\frac{3\hbar}{2m\omega}} \qquad\qquad \sigma_p = \sqrt{\langle p^2\rangle} = \sqrt{\frac{3\hbar}{2m\omega}}$$

Now combining these two we get

$$\boxed{\sigma_x\sigma_p = \sqrt{\frac{3\hbar}{2m\omega}}\sqrt{\frac{3\hbar m\omega}{2}} = \frac{3\hbar}{2} \quad \checkmark}$$

This answer is greater than $\frac{\hbar}{2}$ which is the requirement of the Heisenberg uncertainty principle.

5.6 Computing Kinetic and Potential Energy

By definition

$$\langle T\rangle = \frac{\langle p^2\rangle}{2m}$$

Hence, we can just divide our answer for momentum squared by $2m$ to obtain kinetic energy. For the ground state the kinetic energy is

$$\boxed{\langle T\rangle_0 = \frac{\langle p^2\rangle_0}{2m} = \frac{\frac{\hbar m\omega}{2}}{2m} = \frac{\hbar\omega}{4}}$$

And for the first excited state the kinetic energy is

$$\boxed{\langle T\rangle_1 = \frac{\langle p^2\rangle_1}{2m} = \frac{\frac{3\hbar m\omega}{2}}{2m} = \frac{3\hbar\omega}{4}}$$

The potential is defined as

$$\langle V\rangle = \frac{1}{2}m\omega^2\langle x^2\rangle$$

Therefore, all we have to do is multiply our position squared by $1/2m\omega$ to obtain the potential. For the ground state it is

$$\boxed{\langle V\rangle_0 = \frac{1}{2}m\omega^2\langle x^2\rangle_0 = \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega} = \frac{\hbar\omega}{4}}$$

and for the first excited state

$$\boxed{\langle V\rangle_1 = \frac{1}{2}m\omega^2\langle x^2\rangle_1 = \frac{1}{2}m\omega^2\frac{3\hbar}{2m\omega} = \frac{3\hbar\omega}{4}}$$

The total energy $\langle H\rangle$ is just

$$\langle H\rangle = \langle T\rangle + \langle V\rangle$$

So for the ground state is just

$$\boxed{\langle H\rangle_0 = \langle T\rangle_0 + \langle V\rangle_0 = \frac{\hbar\omega}{4} + \frac{\hbar\omega}{4} = \frac{\hbar\omega}{2}}$$

Which is expected since the energy is given by $(n + \frac{1}{2})\hbar\omega$ and the ground state is $n = 0$. For the first excited state the energy is

$$\boxed{\langle H\rangle_1 = \langle T\rangle_1 + \langle V\rangle_1 = \frac{3\hbar\omega}{4} + \frac{3\hbar\omega}{4} = \frac{3\hbar\omega}{2}}$$

Which is what we would expect since the first excited state is the $n = 1$ state.