Chem 542 Problem Set 9

Questions 1-3 are about a quantum particle on a flat surface

1. A wavepacket $\psi(x) = \left(\frac{1}{2\pi\langle\Delta\hat{x}^2\rangle}\right)^{\frac{1}{4}} e^{\frac{-(x-\langle\hat{x}\rangle)^2}{4\langle\Delta\hat{x}^2\rangle}+\frac{i}{\hbar}\cdot x\cdot\langle\hat{p}\rangle}$ is placed on a flat potential energy surface, meaning $\widehat{H}(\hat{p}) = \frac{\hat{p}_s^2}{2m}$, where $\hat{p}_s$ is the "regular" momentum operator: $\hat{p}_s = -i\hbar\frac{\partial}{\partial x}$ in the Schrodinger frame. Please calculate:

a) $\langle\hat{p}(t)\rangle^2$ **b)** $\langle\hat{p}(t)^2\rangle$ **c)** $\langle\Delta\hat{p}(t)^2\rangle = \langle\hat{p}(t)^2\rangle - \langle\hat{p}(t)\rangle^2$

using the Heisenberg picture. Note that the operator for $\hat{p}(t)$ has to be derived, but your book can guide you on this part.

Answer: a) First, we put the operators into the Heisenberg form:

$$\frac{\partial\hat{p}(t)}{\partial t} = \frac{1}{i\hbar}\left[\hat{p}(t), \widehat{H}(\hat{p})\right]$$

From class we know that $\left[\hat{p}(t), \widehat{H}(\hat{p})\right] = i\hbar\frac{\partial\widehat{H}(\hat{p})}{\partial\hat{x}} = i\hbar\frac{\partial}{\partial\hat{x}}\frac{\hat{p}_s^2}{2m} = 0$. Plugging this into the above yields $\frac{\partial\hat{p}(t)}{\partial t} = 0$. We can integrate to solve for $\hat{p}(t)$:

$\int_{\hat{p}(0)}^{\hat{p}(t)}\partial\hat{p}(t)' = \hat{p}(t) - \hat{p}(0) = 0$ and thus $\hat{p}(t) = \hat{p}(0)$, where $\hat{p}(0)$ is just the position operator in the Schrodinger frame, i.e. $\hat{p}_s = -i\hbar\frac{\partial}{\partial x}$. As a result,

$$\langle\hat{p}(t)\rangle = -i\hbar\int_{-\infty}^{\infty}\psi(x)^*\frac{\partial}{\partial x}\psi(x)\cdot\partial x = \langle\hat{p}\rangle$$

And as a result: $\langle\hat{p}(t)\rangle^2 = \langle\hat{p}\rangle^2$.

b) Likewise,

$$\langle\hat{p}_s^2\rangle = -\hbar^2\int_{-\infty}^{\infty}\psi(x)^*\frac{\partial^2}{\partial x^2}\psi(x)\cdot\partial x = \frac{\hbar^2}{4\langle\Delta x^2\rangle} + \langle\hat{p}\rangle^2$$

c) Thus $\langle\Delta\hat{p}(t)^2\rangle = \langle\hat{p}(t)^2\rangle - \langle\hat{p}(t)\rangle^2 = \frac{\hbar^2}{4\langle\Delta x^2\rangle} + \langle\hat{p}\rangle^2 - \langle\hat{p}\rangle = \frac{\hbar^2}{4\langle\Delta x^2\rangle}$.

This makes sense because the definition of a minimum uncertainty wavepacket requires: $\langle\Delta\hat{p}^2\rangle\langle\Delta x^2\rangle = \frac{\hbar^2}{4}$.

2. For the free particle wavepacket $\psi(x) = \left(\frac{1}{2\pi\langle\Delta\hat{x}^2\rangle}\right)^{\frac{1}{4}} e^{\frac{-(x-\langle\hat{x}\rangle)^2}{4\langle\Delta\hat{x}^2\rangle}+\frac{i}{\hbar}\cdot x\cdot\langle\hat{p}\rangle}$, calculate:

a) $\langle\hat{x}(t)\rangle^2$ **b)** $\langle\hat{x}(t)^2\rangle$ **c)** $\langle\Delta\hat{x}(t)^2\rangle = \langle\hat{x}(t)^2\rangle - \langle\hat{x}(t)\rangle^2$

using the Heisenberg picture. Note that for a free particle $\hat{H}(\hat{p}) = \frac{\hat{p}_s^2}{2m}$, where $\hat{p}_s$ is the "regular" momentum operator in the Schrodinger frame. Note that the operator for $\hat{x}(t)$ has to be derived, but your book can guide you on this part.

Answer: a) First, we put the operators into the Heisenberg form:

$$\frac{\partial \hat{x}(t)}{\partial t} = \frac{1}{i\hbar}\left[\hat{x}(t), \hat{H}(\hat{p})\right]$$

From class we know that $\left[\hat{x}(t), \hat{H}(\hat{p})\right] = i\hbar \frac{\partial \hat{H}(\hat{p})}{\partial \hat{p}} = i\hbar \frac{\partial}{\partial \hat{p}} \frac{\hat{p}_s^2}{2m} = i\hbar \frac{\hat{p}_s}{m}$. Plugging this into the above yields $\frac{\partial \hat{x}(t)}{\partial t} = \frac{1}{i\hbar}\left[\hat{x}(t), \hat{H}(\hat{p})\right] = \frac{1}{i\hbar} i\hbar \frac{\hat{p}_s}{m} = \frac{\hat{p}_s}{m}$. Since $\hat{p}_s$ has no time dependence, we can integrate it easily to solve for $\hat{x}(t)$:

$$\int_{\hat{x}(0)}^{\hat{x}(t)} \partial \hat{x}(t)' = \hat{x}(t) - \hat{x}(0) = \int_0^t \frac{\hat{p}_s}{m} \partial t' = \frac{\hat{p}_s}{m} t$$

Since $\hat{x}(0)$ is just the position operator in the Schrodinger frame, i.e. $\hat{x}_s = x$, we are left with:

$$\hat{x}(t) = \frac{\hat{p}_s}{m} t + \hat{x}_s$$

Now the average position is determined via:

$$\langle \hat{x}(t) \rangle = \int_{-\infty}^{\infty} \psi(x)^* \left\{\frac{\hat{p}_s}{m} t + \hat{x}_s\right\} \psi(x) \cdot \partial x$$

$$= -i\hbar \frac{t}{m} \int_{-\infty}^{\infty} \psi(x)^* \frac{\partial}{\partial x} \psi(x) \cdot \partial x + \int_{-\infty}^{\infty} \psi(x)^* \cdot x \cdot \psi(x) \cdot \partial x$$

We need to use Mathematica to solve this equation; see the accompanying notebook that shows:

$$\langle \frac{\hat{p}_s}{m} t \rangle = -i\hbar \frac{t}{m} \int_{-\infty}^{\infty} \psi(x)^* \frac{\partial}{\partial x} \psi(x) \cdot \partial x = \frac{t}{m} \langle \hat{p} \rangle$$

and:

$$\langle \hat{x}_s \rangle = \int_{-\infty}^{\infty} \psi(x)^* \cdot x \cdot \psi(x) \cdot \partial x = \langle \hat{x} \rangle$$

Thus, $\langle \hat{x}(t) \rangle^2 = \left(\frac{t}{m} \langle \hat{p} \rangle + \langle \hat{x} \rangle\right)^2 = \frac{t^2}{m^2} \langle \hat{p} \rangle^2 + 2\frac{t}{m} \langle \hat{p} \rangle \langle \hat{x} \rangle + \langle \hat{x} \rangle^2$.

b) Next, we tackle $\langle \hat{x}(t)^2 \rangle$. First, expand the operator:

$$\left\{\frac{\hat{p}_s}{m} t + \hat{x}_s\right\}^2 = \frac{t^2}{m^2}\hat{p}_s^2 + \frac{\hat{p}_s}{m} t \cdot \hat{x}_s + \hat{x}_s \cdot \frac{\hat{p}_s}{m} t + \hat{x}_s^2$$

Note that $\hat{p}_s^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$ and using Mathematica we find:

$$\langle \frac{t^2}{m^2}\hat{p}_s^2 \rangle = \frac{t^2}{m^2}\langle \hat{p}_s^2 \rangle = -\hbar^2 \frac{t^2}{m^2} \int_{-\infty}^{\infty} \psi(x)^* \frac{\partial^2}{\partial x^2}\psi(x) \cdot \partial x = \frac{t^2}{m^2}\frac{\hbar^2}{4\langle \Delta x^2 \rangle} + \frac{t^2}{m^2}\langle \hat{p} \rangle^2$$

Likewise: $\langle \frac{\hat{p}_s}{m} t \cdot \hat{x}_s + \hat{x}_s \cdot \frac{\hat{p}_s}{m} t \rangle = \frac{t}{m}\langle \hat{x}_s \hat{p}_s + \hat{p}_s \hat{x}_s \rangle = -i\hbar \frac{t}{m}\langle \hat{x}_s \frac{\partial}{\partial x} + \frac{\partial}{\partial x}\hat{x}_s \rangle =$

$$-i\hbar \frac{t}{m} \int_{-\infty}^{\infty} \psi(x)^* \left\{ x \frac{\partial}{\partial x} + \frac{\partial}{\partial x} x \right\} \psi(x) \cdot \partial x = 2\frac{t}{m}\langle \hat{p} \rangle \langle \hat{x} \rangle$$

Based on the accompanying Mathematica notebook. Last,

$$\langle \hat{x}_s^2 \rangle = \int_{-\infty}^{\infty} \psi(x)^* \cdot x^2 \cdot \psi(x) \cdot \partial x = \langle \Delta \hat{x}^2 \rangle + \langle \hat{x} \rangle^2$$

c) Putting this all together:

$$\begin{aligned} \langle \Delta \hat{x}(t)^2 \rangle &= \langle \hat{x}(t)^2 \rangle - \langle \hat{x}(t) \rangle^2 \\ &= \left(\frac{t^2}{m^2}\frac{\hbar^2}{4\langle \Delta x^2 \rangle} + \frac{t^2}{m^2}\langle \hat{p} \rangle^2 + 2\frac{t}{m}\langle \hat{p} \rangle \langle \hat{x} \rangle + \langle \Delta \hat{x}^2 \rangle + \langle \hat{x} \rangle^2 \right) \\ &+ \left(-\frac{t^2}{m^2}\langle \hat{p} \rangle^2 - 2\frac{t}{m}\langle \hat{p} \rangle \langle \hat{x} \rangle - \langle \hat{x} \rangle^2 \right) = \frac{t^2}{m^2}\frac{\hbar^2}{4\langle \Delta x^2 \rangle} + \langle \Delta \hat{x}^2 \rangle \end{aligned}$$

3. Can you show that $\langle \Delta \hat{p}(t)^2 \rangle \langle \Delta \hat{x}(t)^2 \rangle = \frac{t^2}{m^2}\frac{\hbar^4}{16\langle \Delta x^2 \rangle^2} + \frac{\hbar^2}{4}$?

Answer: Previously we showed that $\langle \Delta \hat{p}(t)^2 \rangle = \frac{\hbar^2}{4\langle \Delta x^2 \rangle}$, and thus:

$$\langle \Delta \hat{p}(t)^2 \rangle \langle \Delta \hat{x}(t)^2 \rangle = \frac{t^2}{m^2}\frac{\hbar^4}{16\langle \Delta x^2 \rangle^2} + \frac{\hbar^2}{4}$$

Questions 4-6 are about a free falling quantum particle

4. Let's say a particle is in a gravitational field, the potential energy operator for which is:

$$\hat{V}(z) = mg \cdot \hat{z}$$

where m is mass and g is the gravitational constant. Note that we usually think of "z" as the up-down direction, whereas we are used to using "x" so be careful!

The total Hamiltonian is: $\hat{H}(t) = \hat{H}(0) = \frac{\hat{p}_s^2}{2m} + mg \cdot \hat{z}_s$, where $\hat{z}_s$ and $\hat{p}_s$ are the "regular" operators: $\hat{z}_s = z$ and $\hat{p}_s = -i\hbar\frac{\partial}{\partial z}$ in the non-time evolving Schrodinger frame. Clearly the Hamiltonian is time-independent.

a) For this system can you solve the Heisenberg operator $\hat{p}(t)$? ***Hint***, the commutator with $\hat{p}$ and $\hat{z}$ in the non-time evolving (Schrodinger frame) is: $[\hat{p}_s, \hat{z}_s] = -i\hbar$.

b) Now solve for $\hat{z}(t)$. ***Hint:*** you will need to incorporate the result from pt. a, and you need to know the identity $[\hat{z}_s, \hat{p}_s^2] = 2i\hbar \cdot \hat{p}_s$.

Double Hint: The solution to this problem won't be like the free particle operators, rather, you will need to think about the spin operator example where you have a coupled differential equation.

Answer: a. We will first solve for $\hat{p}(t)$, for which:

$$\frac{\partial \hat{p}(t)}{\partial t} = \frac{1}{i\hbar}\left[\hat{p}(t), \hat{H}(\hat{p}_S, \hat{z}_S)\right] = \frac{1}{i\hbar}\left[\hat{p}(t), \frac{\hat{p}_S^2}{2m} + mg \cdot \hat{z}_S\right]$$

First, we will factor out the Unitary operators from: $\hat{p}(t) = e^{i\hat{H}t/\hbar} \cdot \hat{p}_S \cdot e^{-i\hat{H}t/\hbar}$:

$$\frac{\partial \hat{p}(t)}{\partial t} = \frac{e^{i\hat{H}t/\hbar}}{i\hbar}\left[\hat{p}_S, \frac{\hat{p}_S^2}{2m} + mg \cdot \hat{z}_S\right] e^{-i\hat{H}t/\hbar}$$

As $\hat{p}_s$ commutes with $\frac{\hat{p}_s^2}{2m}$ (obviously), the problem is:

$$\frac{\partial \hat{p}(t)}{\partial t} = \frac{e^{i\hat{H}t/\hbar}}{i\hbar}[\hat{p}_S, mg \cdot \hat{z}_S]e^{-i\hat{H}t/\hbar}$$

Since $[\hat{p}_s, \hat{z}_S] = -i\hbar$, then: $[\hat{p}_S, \mathrm{mg} \cdot \hat{z}_S] = -i\hbar \cdot mg$, and:

$$\frac{\partial \hat{p}(t)}{\partial t} = \frac{e^{i\hat{H}t/\hbar}}{i\hbar} \cdot -i\hbar \cdot mg \cdot e^{-i\hat{H}t/\hbar} = -mg$$

Now we can solve $\hat{p}(t)$ via:

$$\int_{\hat{p}(0)}^{\hat{p}(t)} \partial\hat{p}(t) = \int_0^t -mg\cdot\partial t$$

Therefore: $\hat{p}(t) = \hat{p}_S - mgt$.

b. First, $\frac{\partial\hat{z}(t)}{\partial t} = \frac{1}{i\hbar}\left[\hat{z}(t), \widehat{H}(\hat{p}_S, \hat{z}_S)\right] = \frac{1}{i\hbar}\left[\hat{z}(t), \frac{\hat{p}_S^2}{2m} + mg\cdot\hat{z}_S\right]$. Next, we have to factor out the Unitary operators that are part of $\hat{x}(t)$ as:

$$\frac{\partial\hat{z}(t)}{\partial t} = \frac{1}{i\hbar}\left[\hat{z}(t), \widehat{H}(\hat{p}_S, \hat{z}_S)\right] = \frac{e^{i\widehat{H}t/\hbar}}{i\hbar}\left[\hat{z}_S, \frac{\hat{p}_S^2}{2m} + mg\cdot\hat{z}_S\right]e^{-i\widehat{H}t/\hbar}$$

Clearly $\hat{z}_S$ commutes with $mg\cdot\hat{z}_S$, so the problem is:

$$\frac{\partial\hat{z}(t)}{\partial t} = \frac{e^{i\widehat{H}t/\hbar}}{i\hbar}\left[\hat{z}_S, \frac{{\hat{p}_S}^2}{2m}\right]e^{-i\widehat{H}t/\hbar}$$

We have reviewed this problem before, so we know that $\left[\hat{z}_S, \frac{{\hat{p}_S}^2}{2m}\right] = \frac{i\hbar\cdot\hat{p}_S}{m}$, which means:

$$\frac{\partial\hat{z}(t)}{\partial t} = \frac{1}{m}e^{i\widehat{H}t/\hbar}\cdot\hat{p}_S\cdot e^{-i\widehat{H}t/\hbar} = \frac{\hat{p}(t)}{m}$$

Since we already know $\hat{p}(t) = \hat{p}_S - mgt$ then:

$$\frac{\partial\hat{z}(t)}{\partial t} = \frac{\hat{p}(t)}{m} = \frac{\hat{p}_S}{m} - gt$$

And therefore

$$\int_{\hat{z}_S}^{\hat{z}(t)} \partial\hat{z}(t) = \int_0^t \left(\frac{\hat{p}_S}{m} - gt\right)\cdot\partial t$$

Therefore $\hat{z}(t) = \hat{z}_S + \frac{t}{m}\hat{p}_S - \frac{g\cdot t^2}{2}$

5. For the free particle wavepacket in a gravitational field:

$$\psi(z) = \left(\frac{1}{2\pi\langle\Delta\hat{z}^2\rangle}\right)^{\frac{1}{4}} e^{\frac{-(z-\langle\hat{z}\rangle)^2}{4\langle\Delta\hat{z}^2\rangle}+\frac{i}{\hbar}z\cdot\langle\hat{p}\rangle}$$

calculate: **a)** $\langle\hat{p}(t)\rangle^2$ **b)** $\langle\hat{p}(t)^2\rangle$ **c)** $\langle\Delta\hat{p}(t)^2\rangle = \langle\hat{p}(t)^2\rangle - \langle\hat{p}(t)\rangle^2$

Answer:

a) First, we put the operators into the Heisenberg form:

$$\langle \hat{p}(t) \rangle = \int_{-\infty}^{\infty} \psi(z)^* \left(\hat{p}_S - mg \cdot t\right)\psi(z) \cdot \partial z$$

$$= \int_{-\infty}^{\infty} \psi(z)^* \left(-i\hbar\right)\frac{\partial}{\partial z}\psi(z) \cdot \partial z - \int_{-\infty}^{\infty} \psi(z)^* \left(mg \cdot t\right)\psi(z) \cdot \partial z = \langle \hat{p} \rangle - mgt$$

where we used Mathematica to solve: $\int_{-\infty}^{\infty} \psi(z)^*(-i\hbar)\frac{\partial}{\partial z}\psi(z) \cdot \partial z = \langle \hat{p} \rangle$:

```
In[∘]:= Integrate[Conjugate[f[x]] * (-ⅈ * h) * D[f[x], x], {x, -Infinity, Infinity},
         Assumptions → {h > 0, dXsq > 0, avex > 0, avep > 0}]
Out[∘]= avep
```

Note that we need to know $\langle \hat{p}(t) \rangle^2$ for the final answer, which is clearly:

$$\langle \hat{p}(t) \rangle^2 = \left(\langle \hat{p} \rangle - mgt\right)^2 = \langle \hat{p} \rangle^2 - 2\langle \hat{p} \rangle \cdot mgt + (mgt)^2$$

b) Likewise, $\hat{p}(t)^2 = \left(\hat{p}(0) - mgt\right)^2 = \hat{p}(0)^2 - 2 \cdot mgt \cdot \hat{p}(0) + (mgt)^2$

Hence:

$$\langle \hat{p}(t)^2 \rangle = \int_{-\infty}^{\infty} \psi(z)^* \left\{\hat{p}_S^2 - 2 \cdot mgt \cdot \hat{p}_S + (mgt)^2\right\}\psi(z) \cdot \partial z$$

$$= \int_{-\infty}^{\infty} \psi(z)^* \cdot \hat{p}_S^2 \cdot \psi(z) \cdot \partial z - 2mgt \cdot \int_{-\infty}^{\infty} \psi(z)^* \left(-i\hbar\right)\frac{\partial}{\partial z}\psi(z) \cdot \partial z$$

$$+ (mgt)^2 \int_{-\infty}^{\infty} \psi(z)^* \psi(z) \cdot \partial z$$

It should be clear from pt. a that:

$$-2mgt \cdot \int_{-\infty}^{\infty} \psi(z)^*(-i\hbar)\frac{\partial}{\partial z}\psi(z) \cdot \partial z = -2 \cdot mgt \cdot \langle \hat{p} \rangle$$

and since $(mgt)^2$ are constants: $(mgt)^2 \int_{-\infty}^{\infty} \psi(z)^* \psi(z) \cdot \partial z = (mgt)^2$

The only thing to use Mathematica for is $\langle \hat{p}_S^2 \rangle = \langle -\hbar^2 \frac{\partial^2}{\partial z^2} \rangle$:

$$\langle \hat{p}_S^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi(z)^* \frac{\partial^2}{\partial z^2}\psi(z) \cdot \partial z = \frac{\hbar^2}{4\langle \Delta z^2 \rangle} + \langle \hat{p} \rangle^2$$

as shown below:

In[ ]:=
```
Integrate[Conjugate[f[x]] * (-h * h) * D[D[f[x], x], x], {x, -Infinity, Infinity},
 Assumptions → {h > 0, dXsq > 0, avex > 0, avep > 0}]
```

Out[ ]= $\text{avep}^2 + \frac{h^2}{4\ \text{dXsq}}$

c) Thus:

$$\langle(\Delta\hat{p}(t))^2\rangle = \langle\hat{p}(t)^2\rangle - \langle\hat{p}(t)\rangle^2 =$$

$$\frac{\hbar^2}{4\langle\Delta z^2\rangle} + \langle\hat{p}\rangle^2 - 2\cdot mgt\cdot\langle\hat{p}\rangle + (mgt)^2 - \langle\hat{p}\rangle^2 + 2\langle\hat{p}\rangle\cdot mgt - (mgt)^2 = \frac{\hbar^2}{4\langle\Delta z^2\rangle}$$

6. Worked out for you in the appendix is: $\langle(\Delta\hat{z}(t))^2\rangle = \langle\Delta\hat{z}^2\rangle + \frac{\hbar^2\cdot t^2}{4\langle\Delta z^2\rangle m^2}$

Can you show that $\langle\Delta\hat{p}(t)^2\rangle\langle\Delta\hat{z}(t)^2\rangle = \frac{\hbar^2}{4} + \frac{\hbar^4\cdot t^2}{16\langle\Delta\hat{z}^2\rangle^2 m^2}$?

Answer: Previously we showed that $\langle\Delta\hat{p}(t)^2\rangle = \frac{\hbar^2}{4\langle\Delta z^2\rangle}$, and thus:

$$\langle\Delta\hat{p}(t)^2\rangle\langle\Delta\hat{z}(t)^2\rangle = \frac{\hbar^2}{4\langle\Delta\hat{z}^2\rangle}\left(\langle\Delta\hat{z}^2\rangle + \frac{\hbar^2\cdot t^2}{4\langle\Delta\hat{z}^2\rangle m^2}\right) = \frac{\hbar^2}{4} + \frac{\hbar^4\cdot t^2}{16\langle\Delta\hat{z}^2\rangle^2 m^2}$$

Appendix

Derivation of the identity in question 6:

For the free particle wavepacket $\psi(z) = \left(\frac{1}{2\pi\langle\Delta\hat{z}^2\rangle}\right)^{\frac{1}{4}} e^{\frac{-(z-\langle\hat{z}\rangle)^2}{4\langle\Delta\hat{z}^2\rangle}+\frac{i}{\hbar}\cdot z\cdot\langle\hat{p}\rangle}$, we will show that

$$\langle\Delta\hat{z}(t)^2\rangle = \langle\hat{z}(t)^2\rangle - \langle\hat{z}(t)\rangle^2 = \langle\Delta\hat{z}^2\rangle + \frac{\hbar^2\cdot t^2}{4\langle\Delta z^2\rangle m^2}$$

in a gravitational field.

First, we start with $\langle\hat{z}(t)\rangle$ using $\hat{z}(t) = \hat{z}_s + \frac{t}{m}\hat{p}_s - \frac{gt^2}{2}$:

$$\langle\hat{z}(t)\rangle = \int_{-\infty}^{\infty} \psi(z)^* \left(\hat{z}_s + \frac{t}{m}\hat{p}_s - \frac{g\cdot t^2}{2}\right)\psi(z)\cdot\partial z$$

$$= \int_{-\infty}^{\infty} \psi(z)^*\cdot z\cdot\psi(z)\cdot\partial z + \frac{t}{m}\int_{-\infty}^{\infty} \psi(z)^*\cdot\hat{p}_s\cdot\psi(z)\cdot\partial z - \left(\frac{gt^2}{2}\right)\int_{-\infty}^{\infty}\psi(z)^*\cdot\psi(z)\cdot\partial z$$

We use Mathematica to solve the 1st term: $\int_{-\infty}^{\infty}\psi(z)^*\cdot z\cdot\psi(z)\cdot\partial z = \langle\hat{z}\rangle$ as shown:

```
In[∘]:= f[x] = (1/(2*Pi*dXsq))^(1/4)*Exp[-(1/4/dXsq)*(x-avex)^2+ⅈ/h*x*avep]
```

Out[∘]= $\frac{\left(\frac{1}{dXsq}\right)^{1/4} e^{\frac{i\, avep\, x}{h}-\frac{(-avex+x)^2}{4\, dXsq}}}{(2\pi)^{1/4}}$

```
In[∘]:= Integrate[Conjugate[f[x]]*x*f[x], {x, -Infinity, Infinity},
         Assumptions → {h > 0, dXsq > 0, avex > 0, avep > 0}]
```

Out[∘]= avex

As part of the question you show that $\int_{-\infty}^{\infty}\psi(z)^*\cdot\hat{p}_s\cdot\psi(z)\cdot\partial z = \langle\hat{p}\rangle$, thus:

$$\frac{t}{m}\int_{-\infty}^{\infty}\psi(z)^*\cdot\left\{-i\hbar\frac{\partial}{\partial z}\right\}\cdot\psi(z)\cdot\partial z = \frac{\langle\hat{p}\rangle\cdot t}{m}$$

and due to the fact that $\frac{g\cdot t^2}{2m}$ are just constants:

$$\left(\frac{gt^2}{2}\right)\int_{-\infty}^{\infty}\psi(z)^*\cdot\psi(z)\cdot\partial z = \frac{gt^2}{2}$$

As a result:

$$\langle\hat{z}(t)\rangle^2 = \left(\langle\hat{z}\rangle + \frac{\langle\hat{p}\rangle\cdot t}{m} - \frac{gt^2}{2}\right)^2 = \langle\hat{z}\rangle^2 + \frac{2\langle\hat{z}\rangle\langle\hat{p}\rangle\cdot t}{m} - g\langle\hat{z}\rangle t^2 + \frac{\langle\hat{p}\rangle^2\cdot t^2}{m^2} - \frac{g\langle\hat{p}\rangle\cdot t^3}{m} + \left(\frac{gt^2}{2}\right)^2$$

Next we solve $\langle \hat{z}(t)^2 \rangle$ using:

$$\hat{z}(t)^2 = \left(\hat{z}_s + \frac{t}{m}\hat{p}_s - \frac{gt^2}{2}\right)^2$$

$$= \hat{z}_s^2 + \frac{t}{m}\hat{z}_s \cdot \hat{p}_s + \frac{t}{m}\hat{p}_s \cdot \hat{z}_s - gt^2\hat{z}_s + \frac{t^2}{m^2}\hat{p}_s^2 - \frac{gt^3}{m}\hat{p}_s + \left(\frac{gt^2}{2}\right)^2$$

Most of the terms in $\langle \hat{z}(t)^2 \rangle$ can be solved with no need to do any real evaluation, especially when we use results from question 3 such as $\langle \hat{p}(0)^2 \rangle = \frac{\hbar^2}{4\langle \Delta z^2 \rangle} + \langle \hat{p} \rangle^2$:

$$-\int_{-\infty}^{\infty} \psi(z)^* \cdot (gt^2 \cdot \hat{z}_s) \cdot \psi(z) \cdot \partial z = -g\langle \hat{z} \rangle t^2$$

$$\int_{-\infty}^{\infty} \psi(z)^* \cdot \left(\frac{t^2}{m^2}\hat{p}_s^2\right) \cdot \psi(z) \cdot \partial z = \frac{\hbar^2 \cdot t^2}{4\langle \Delta z^2 \rangle m^2} + \frac{\langle \hat{p} \rangle^2 \cdot t^2}{m^2}$$

$$-\int_{-\infty}^{\infty} \psi(z)^* \cdot \left(\frac{gt^3}{m}\hat{p}_s\right) \cdot \psi(z) \cdot \partial z = -\frac{g\langle \hat{p} \rangle t^3}{m}$$

$$\int_{-\infty}^{\infty} \psi(z)^* \cdot \left(\frac{gt^2}{2}\right)^2 \cdot \psi(z) \cdot \partial z = \left(\frac{gt^2}{2}\right)^2$$

The only terms needing evaluation are:

$$\int_{-\infty}^{\infty} \psi(z)^* \cdot \hat{z}(0)^2 \cdot \psi(z) \cdot \partial z = \langle \hat{z} \rangle^2 + \langle \Delta \hat{z}^2 \rangle$$

```
In[∘]:= Integrate[Conjugate[f[x]] * x * x * f[x], {x, -Infinity, Infinity},
         Assumptions → {h > 0, dXsq > 0, avex > 0, avep > 0}]

Out[∘]= avex^2 + dXsq
```

and:

$$\int_{-\infty}^{\infty} \psi(z)^* \cdot \left(\frac{t}{m} \cdot \hat{z}_s\hat{p}_s\right) \cdot \psi(z) \cdot \partial z = -\frac{i\hbar \cdot t}{m}\int_{-\infty}^{\infty} \psi(z)^* \cdot z \cdot \frac{\partial}{\partial z} \cdot \psi(z) \cdot \partial z = \frac{i\hbar \cdot t}{2m} - \frac{i^2\hbar \cdot t}{m}\frac{\langle \hat{p} \rangle \langle \hat{z} \rangle}{\hbar}$$

$$= \frac{i\hbar \cdot t}{2m} + \frac{\langle \hat{p} \rangle \langle \hat{z} \rangle \cdot t}{m}$$

The above is from the following Mathematica script:

```
In[•]:= -ⅈ*h*t/m*Integrate[Conjugate[f[x]]*x*D[f[x], x], {x, -Infinity, Infinity},
        Assumptions → {h > 0, dXsq > 0, avex > 0, avep > 0}]
```

$$Out[\circ]= -\frac{\mathbb{i}\left(-\frac{1}{2}+\frac{\mathbb{i}\,\text{avep avex}}{h}\right) h\,t}{m}$$

Likewise:

$$\int_{-\infty}^{\infty}\psi(z)^*\cdot\left(\frac{t}{m}\cdot\hat{p}_s\hat{z}_s\right)\cdot\psi(z)\cdot\partial z=-\frac{i\hbar\cdot t}{m}\int_{-\infty}^{\infty}\psi(z)^*\cdot\frac{\partial}{\partial z}z\cdot\psi(z)\cdot\partial z$$

$$=-\frac{i\hbar\cdot t}{2m}-\frac{i^2\hbar\cdot t\cdot\langle\hat{p}\rangle\langle\hat{z}\rangle}{m\hbar}=-\frac{i\hbar\cdot t}{2m}+\frac{\langle\hat{p}\rangle\langle\hat{z}\rangle\cdot t}{m}$$

```
In[•]:= -ⅈ*h*t/m*Integrate[Conjugate[f[x]]*D[x*f[x], x], {x, -Infinity, Infinity},
        Assumptions → {h > 0, dXsq > 0, avex > 0, avep > 0}]
```

$$Out[\circ]= -\frac{\mathbb{i}\left(\frac{1}{2}+\frac{\mathbb{i}\,\text{avep avex}}{h}\right) h\,t}{m}$$

Putting this all together:

$$\langle\hat{z}(t)^2\rangle=\langle\hat{z}\rangle^2+\langle\Delta\hat{z}^2\rangle+\frac{i\hbar\cdot t}{2m}+\frac{\langle\hat{p}\rangle\langle\hat{z}\rangle\cdot t}{m}-\frac{i\hbar\cdot t}{2m}+\frac{\langle\hat{p}\rangle\langle\hat{z}\rangle\cdot t}{m}-g\langle\hat{z}\rangle\cdot t^2+\frac{\hbar^2\cdot t^2}{4\langle\Delta z^2\rangle m^2}$$
$$+\frac{\langle\hat{p}\rangle^2\cdot t^2}{m^2}-\frac{\langle\hat{p}\rangle g t^3}{m}+\left(\frac{gt^2}{2}\right)^2$$

$$=\langle\hat{z}\rangle^2+\langle\Delta\hat{z}^2\rangle+\frac{2\langle\hat{p}\rangle\langle\hat{z}\rangle\cdot t}{m}-g\langle\hat{z}\rangle t^2+\frac{\hbar^2\cdot t^2}{4\langle\Delta z^2\rangle m^2}+\frac{\langle\hat{p}\rangle^2\cdot t^2}{m^2}-\frac{\langle\hat{p}\rangle\cdot g t^3}{m}+\left(\frac{gt^2}{2}\right)^2$$

Hence:

$$\langle\Delta\hat{z}(t)^2\rangle=\langle\hat{z}(t)^2\rangle-\langle\hat{z}(t)\rangle^2=$$

$$\langle\hat{z}\rangle^2+\langle\Delta\hat{z}^2\rangle+\frac{2\langle\hat{p}\rangle\langle\hat{z}\rangle\cdot t}{m}-g\langle\hat{z}\rangle\cdot t^2+\frac{\hbar^2\cdot t^2}{4\langle\Delta z^2\rangle m^2}+\frac{\langle\hat{p}\rangle^2\cdot t^2}{m^2}-\frac{g\langle\hat{p}\rangle\cdot t^3}{m}+\left(\frac{gt^2}{2}\right)^2$$

$$-\langle\hat{z}\rangle^2-\frac{2\langle\hat{z}\rangle\langle\hat{p}\rangle\cdot t}{m}+g\langle\hat{z}\rangle\cdot t^2-\frac{\langle\hat{p}\rangle^2\cdot t^2}{m^2}+\frac{g\langle\hat{p}\rangle\cdot t^3}{m}-\left(\frac{gt^2}{2}\right)^2$$

$$=\langle\Delta\hat{z}^2\rangle+\frac{\hbar^2\cdot t^2}{4\langle\Delta z^2\rangle m^2}$$

Example calculations of the properties of the ground state vibrational wavefunction using Mathematica

Given the normalized wavefunction: $\psi(x) = \left(\frac{m\cdot\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{\frac{-m\cdot\omega\cdot x^2}{2\hbar}}$

```
f[x] = (m * w / Pi / h) ^ (1 / 4) * Exp[-m * w * x * x / 2 / h]
```

Check for normalization: $\int_{-\infty}^{\infty} \psi(x)^* \cdot \psi(x) \cdot \partial x$

In[ ]:=
```
Integrate[Conjugate[f[x]] * f[x], {x, -Infinity, Infinity},
 Assumptions → {m > 0, w > 0, h > 0}]
```

Out[ ]= 1

Calculate the derivative of the wavefunction: $\frac{\partial\psi(x)}{\partial x}$:

In[ ]:=
```
D[f[x], x]
```

Out[ ]= $-\frac{e^{-\frac{m\,w\,x^2}{2\,h}}\, m\, w \left(\frac{m\,w}{h}\right)^{1/4} x}{h\,\pi^{1/4}}$

Calculate the double derivative of the wavefunction: $\frac{\partial^2\psi(x)}{\partial x^2}$:

In[ ]:=
```
D[D[f[x], x], x]
```

Out[ ]= $-\frac{e^{-\frac{m\,w\,x^2}{2\,h}}\, m\, w \left(\frac{m\,w}{h}\right)^{1/4}}{h\,\pi^{1/4}} + \frac{e^{-\frac{m\,w\,x^2}{2\,h}}\, m^2\, w^2 \left(\frac{m\,w}{h}\right)^{1/4} x^2}{h^2\,\pi^{1/4}}$

Average position in the Schrodinger representation: $\langle\hat{x}_s\rangle = \int_{-\infty}^{\infty} \psi(x)^* \cdot x \cdot \psi(x) \cdot \partial x$

In[ ]:=
```
Integrate[Conjugate[f[x]] * x * f[x], {x, -Infinity, Infinity},
 Assumptions → {m > 0, w > 0, h > 0}]
```

Out[ ]= 0

Average position^2 in the Schrodinger representation: $\langle\hat{x}_s^2\rangle = \int_{-\infty}^{\infty} \psi(x)^* \cdot x^2 \cdot \psi(x) \cdot \partial x$

In[ ]:=
```
Integrate[Conjugate[f[x]] * x * x * f[x], {x, -Infinity, Infinity},
 Assumptions → {m > 0, w > 0, h > 0}]
```

Out[ ]= $\frac{h}{2\,m\,w}$

Average momentum in either the Heisenberg or Schrodinger representation:

$\langle \hat{p} \rangle = -i\hbar \int_{-\infty}^{\infty} \psi(x)^* \frac{\partial}{\partial x} \psi(x) \cdot \partial x$:

In[ ]:=
```
-i * h * Integrate[Conjugate[f[x]] * D[f[x], x], {x, -Infinity, Infinity},
  Assumptions → {m > 0, w > 0, h > 0}]
```

Out[ ]= 0

Average momentum^2 in either the Heisenberg or Schrodinger representation:

$\langle \hat{p} \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi(x)^* \frac{\partial^2}{\partial x^2} \psi(x) \cdot \partial x$:

In[ ]:=
```
-h * h * Integrate[Conjugate[f[x]] * D[D[f[x], x], x], {x, -Infinity, Infinity},
  Assumptions → {m > 0, w > 0, h > 0}]
```

Out[ ]= $\frac{\text{h m w}}{2}$

Uncertainty relation $(\langle \hat{x}_s^2 \rangle - \langle \hat{x}_s \rangle)(\langle \hat{p}_s^2 \rangle - \langle \hat{p}_s \rangle) = \left(\frac{\hbar}{2m\omega} - 0\right)\left(\frac{\hbar m\omega}{2} - 0\right) = \frac{\hbar}{4}$