PHYS 23410 (Quantum Mechanics I) Problem Sets

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Contents

1 Formalism of Quantum Mechanics

1/12: **1.** The Schrödinger equation is given by

$$\left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r},t)\right)\psi(\vec{r},t) = i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$

a) Use this equation, and its complex conjugate, to demonstrate the **continuity equation**

$$\frac{\partial|\psi(\vec{r},t)|^2}{\partial t} + \vec{\nabla}\left(\frac{i\hbar}{2m}\right)\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right) = 0$$

where the first term, with $|\psi|^2 = \psi^*\psi$, is the partial derivative of the probability density, while the second term is the divergence of the probability current density.

Answer. Multiply both sides of the Schrödinger equation by $-i/\hbar$:

$$\frac{\partial\psi}{\partial t} = \left(\frac{i\hbar}{2m}\vec{\nabla}^2 - \frac{i}{\hbar}V\right)\psi$$

We may then obtain the complex conjugate of the above equation by replacing all instances of i with its complex conjugate $-i$ and ψ with its complex conjugate ψ^*. In a nutshell, this works because we have a case of multiplying some complex number $a + bi = \psi(\vec{r})$ on the left by i, which gives $i(a + bi) = -b + ai$, and the complex conjugate of this number is $-b - ai = -i(a - bi) = -i(a + bi)^*$.

$$\frac{\partial\psi^*}{\partial t} = \left(-\frac{i\hbar}{2m}\vec{\nabla}^2 + \frac{i}{\hbar}V\right)\psi^*$$

We will use the above two equations to substitute into the following algebraic derivation, which yields the desired result.

$$\begin{aligned}
\frac{\partial|\psi|^2}{\partial t} &= \frac{\partial}{\partial t}(\psi^*\psi) \\
&= \psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t} \\
&= \psi^*\left(\frac{i\hbar}{2m}\vec{\nabla}^2 - \frac{i}{\hbar}V\right)\psi + \psi\left(-\frac{i\hbar}{2m}\vec{\nabla}^2 + \frac{i}{\hbar}V\right)\psi^* \\
&= \frac{i\hbar}{2m}\left(\psi^*\vec{\nabla}^2\psi - \psi\vec{\nabla}^2\psi^*\right) \\
&= \frac{i\hbar}{2m}\left[\left(\vec{\nabla}\psi^*\vec{\nabla}\psi + \psi^*\vec{\nabla}^2\psi\right) - \left(\vec{\nabla}\psi\vec{\nabla}\psi^* + \psi\vec{\nabla}^2\psi^*\right)\right] \\
&= \frac{i\hbar}{2m}\vec{\nabla}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) \\
&= -\vec{\nabla}\left(\frac{i\hbar}{2m}\right)\left(\psi\vec{\nabla}\psi^* - \psi^*\vec{\nabla}\psi\right)
\end{aligned}$$

□

b) Discuss the physical interpretation of this equation. What happens if you integrate the first and second terms over a region of space, defined by a finite volume V and separated by the rest of space by a boundary area S?

Hint: Use the analogy with the case of electromagnetic charge. If you integrate over the whole volume of space, the continuity equation leads to charge conservation. The probability current density, just as the charge current density, is assumed to vanish sufficiently fast at infinity, so that there is no flow of probability (charge) at infinity.

Answer. This equation implies that probability density is *locally* conserved. In its current differential form, it states that the change in probability density (first term) is exactly offset by the divergence or the probability current density (second term). This interpretation is clarified upon integrating over a volume V contained within a boundary surface S. In the integral form, the first term becomes the change in probability density within V, i.e., the rate at which the particle becomes more or less likely to exist within V. Moreover, this is equal to the opposite of the second term, which when integrated gives the flux of the probability density through S. Essentially, if the particle is going to become less likely to exist within V, then a corresponding amount of probability density must flow out of V through S (and vice versa if the particle is going to become more likely to exist within V).

Additionally, note that if you take the limit as $V \to \mathbb{C}^3$, both terms go to zero (because probability density is conserved within the entire space). Since the sum of two terms equal to zero is zero, this is another way of verifying the equality in the continuity equation. □

2. Consider the expectation value of the operator $\hat{\vec{p}}^2 = -\hbar^2 \vec{\nabla}^2$, namely

$$\int \mathrm{d}^3\vec{r}\ \psi(\vec{r},t)^* \left(-\hbar^2\vec{\nabla}^2\psi(\vec{r},t)\right)$$

a) Using integration by parts, demonstrate that this can be rewritten as the integral of the modulus square of the gradient of $\hbar\psi(\vec{r},t)$ and that it is therefore a positive quantity. As before, assume that the wave functions go sufficiently fast to zero at infinity.

Answer. To begin, we need to derive a three-dimensional analogy to the standard one-dimensional integration by parts formula. Let $u, v : \mathbb{C}^3 \to \mathbb{C}^3$ be functions with smoothness constraints analogous to ψ. As in the one-dimensional case, we'll start with the product rule and integrate.

$$\begin{aligned}
\vec{\nabla}\cdot(u\vec{\nabla}v) &= (\vec{\nabla}u)(\vec{\nabla}v) + u\vec{\nabla}^2 v \\
\int_\Omega \vec{\nabla}\cdot(u\vec{\nabla}v) &= \int_\Omega (\vec{\nabla}u)(\vec{\nabla}v) + \int_\Omega u\vec{\nabla}^2 v \\
\int_\Omega \vec{\nabla}\cdot(u\vec{\nabla}v) - \int_\Omega (\vec{\nabla}u)(\vec{\nabla}v) &= \int_\Omega u\vec{\nabla}^2 v
\end{aligned}$$

We can then apply this result and simplify to yield the final result.

$$\begin{aligned}
\int \mathrm{d}^3\vec{r}\ \psi^*\left(-\hbar^2\vec{\nabla}^2\psi\right) &= -\int \mathrm{d}^3\vec{r}\ \underbrace{\hbar\psi^*}_{u}\underbrace{\vec{\nabla}^2(\hbar\psi)}_{\vec{\nabla}^2 v} \\
&= -\underbrace{\int \vec{\nabla}\cdot\left[(\hbar\psi^*)\vec{\nabla}(\hbar\psi)\right]}_{0} + \int \mathrm{d}^3\vec{r}\ \vec{\nabla}(\hbar\psi^*)\vec{\nabla}(\hbar\psi) \\
&= \int \mathrm{d}^3\vec{r}\ |\vec{\nabla}(\hbar\psi)|^2
\end{aligned}$$

To clarify, we know that the first term given by integration by parts goes to zero because of the divergence theorem. In particular, let Ω be a finite region of space encapsulated by $\mathrm{d}\Omega$; we will take the limit as $\Omega \to \mathbb{C}^3$ and $\mathrm{d}\Omega$ approaches the boundary of $\mathbb{C}^3$. Then

$$\int_\Omega \vec{\nabla}\cdot[\hbar\psi^*\vec{\nabla}(\hbar\psi)] = \int_{\mathrm{d}\Omega}[\hbar\psi^*\vec{\nabla}(\hbar\psi)]\cdot\hat{n}\,\mathrm{d}S$$

Essentially, this means that the original integral is equal to an integral of an integrand containing ψ^* (which goes to zero at the "boundary" of $\mathbb{C}^3$) at a surface approaching the boundary through the aforementioned limit. This means that the second integral — under the limit that $\mathrm{d}\Omega$ approaches the "boundary" of $\mathbb{C}^3$ — is zero, justifying the original substitution. □

b) Now consider the expectation value of the Hamiltonian $\hat{\vec{p}}^2/2m + V(\vec{r},t)$ and assume that the function $\psi(\vec{r},t)$ is an eigenfunction of the Hamiltonian. In such a case,

$$\hat{H}\psi(\vec{r},t) = E\psi$$

and the particle therefore has a well-defined energy, equal to E. Demonstrate, based on the result of part (a), that E must be larger than the minimum value of $V(\vec{r},t)$.

Hint: Use $(\hat{\vec{p}}^2/2m)\psi = (E - V)\psi$, and the fact that the mean value of V should be larger than its minimum value.

The lesson is that the particle can enter regions of space where its energy is lower than the potential, but this is not possible everywhere in space. The fact that the particle can go through regions of space where its energy is lower than the potential (the wave function does not vanish in those regions of space) leads to the famous phenomenon of tunneling, namely a particle can go through a *finite region of space where the potential is higher than its energy* and has a probability of being transmitted to the other side.

Answer. Taking the hint, we have that

$$\begin{aligned}
E - \langle V\rangle &= E\cdot 1 - \langle V\rangle \\
&= E\cdot\int \mathrm{d}^3\vec{r}\ \psi^*\psi - \int \mathrm{d}^3\vec{r}\ \psi^* V\psi \\
&= \int \mathrm{d}^3\vec{r}\ \psi^*(E - V)\psi \\
&= \int \mathrm{d}^3\vec{r}\ \psi^*\left(\frac{\hat{\vec{p}}^2}{2m}\right)\psi \\
&= \frac{1}{2m}\int \mathrm{d}^3\vec{r}\ \psi^*(-\hbar^2\vec{\nabla}^2)\psi \\
&= \frac{1}{2m}\int \mathrm{d}^3\vec{r}\ |\vec{\nabla}(\hbar\psi)|^2 && \text{Part (a)} \\
&> 0
\end{aligned}$$

Taking the hint again, we have that

$$\langle V\rangle > V_{\min}$$

Therefore, by transitivity, we have that

$$\begin{aligned}
E - \langle V\rangle &> 0 \\
E > \langle V\rangle &> V_{\min}
\end{aligned}$$

as desired. □

3. We shall define **Hermitian operators** as those ones $\hat{O}$ satisfying the property

$$\int \mathrm{d}^3\vec{r}\ \psi_m^*(\vec{r},t)\hat{O}\psi_n(\vec{r},t) = \left(\int \mathrm{d}^3\vec{r}\ \psi_n^*(\vec{r},t)\hat{O}\psi_m(\vec{r},t)\right)^* \tag{1.1}$$

where ψ_m is a particular solution of the Schrödinger equation. Observe that when you identify $\psi_n = \psi_m$, you obtain that the mean value of a Hermitian operator is real and thus can be associated with an observable.

Observe also that, in general, this could be written as

$$\int \mathrm{d}^3\vec{r}\ \psi_m^*(\vec{r},t)\hat{O}\psi_n(\vec{r},t) = \int \mathrm{d}^3\vec{r}\ [\hat{O}\psi_m(\vec{r},t)]^*\psi_n(\vec{r},t)$$

Therefore, in the case of a Hermitian operator, I can "transfer" the application of the operator from the right to the left.

a) Use this property to demonstrate that if you take two different Hermitian operators and you transfer them in the proper order, then

$$\langle\psi_m|\hat{O}_1\hat{O}_2|\psi_n\rangle = \Big(\langle\psi_n|\hat{O}_2\hat{O}_1|\psi_m\rangle\Big)^*$$

where I used the Dirac notation. Observe that if I take $\hat{O}_2$ to be a real constant, this equation reduces to Equation 1.1.

Answer. We have that

$$\begin{aligned}
\langle\psi_m|\hat{O}_1\hat{O}_2|\psi_n\rangle &= \int \mathrm{d}^3\vec{r}\ \psi_m^*\hat{O}_1\hat{O}_2\psi_n \\
&= \int \mathrm{d}^3\vec{r}\ (\hat{O}_1\psi_m)^*\hat{O}_2\psi_n \\
&= \int \mathrm{d}^3\vec{r}\ [\hat{O}_2(\hat{O}_1\psi_m)]^*\psi_n \\
&= \left(\int \mathrm{d}^3\vec{r}\ \psi_n^*[\hat{O}_2(\hat{O}_1\psi_m)]\right)^* \\
&= \left(\int \mathrm{d}^3\vec{r}\ \psi_n^*\hat{O}_2\hat{O}_1\psi_m\right)^* \\
&= \Big(\langle\psi_n|\hat{O}_2\hat{O}_1|\psi_m\rangle\Big)^*
\end{aligned}$$

as desired. □

b) Use this relation to demonstrate that the mean value of the **commutator** of two Hermitian operators, which is given by

$$[\hat{O}_1,\hat{O}_2] = \hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1$$

is a pure imaginary number, and hence (unless it is multiplied by an imaginary factor), cannot be associated with a physical observable. In the particular example of momentum and position, for instance, $[\hat{p}_i,\hat{r}_j] = -i\hbar\delta_{ij}$, where δ_{ij} is the **Kronecker delta**. Do it for the mean value of the commutator in a particular state with wave function ψ_n.

Answer. We have that

$$\begin{aligned}
\langle\psi|[\hat{O}_1,\hat{O}_2]|\psi\rangle &= \langle\psi|\hat{O}_1\hat{O}_2 - \hat{O}_2\hat{O}_1|\psi\rangle \\
&= \langle\psi|\hat{O}_1\hat{O}_2|\psi\rangle - \langle\psi|\hat{O}_2\hat{O}_1|\psi\rangle \\
&= \underbrace{\langle\psi|\hat{O}_1\hat{O}_2|\psi\rangle}_{a+bi} - (\underbrace{\langle\psi|\hat{O}_1\hat{O}_2|\psi\rangle}_{a-bi})^*
\end{aligned}$$

Since taking the difference of a complex number $a+bi$ and its complex conjugate $a-bi$ yields the purely imaginary number $2bi$, we have the desired result.
Now consider the explicit case where $\hat{O}_1 = \hat{p}_i$, $\hat{O}_2 = \hat{r}_j$, and $\psi = \psi_n$. Then we have that

$$\begin{aligned}
\langle\psi_n|[\hat{p}_i,\hat{r}_j]|\psi_n\rangle &= \langle\psi_n|-i\hbar\delta_{ij}|\psi_n\rangle \\
&= -i\hbar\delta_{ij}\int \mathrm{d}^3\vec{r}\ \psi_n^*\psi_n \\
&= -i\hbar\delta_{ij}\int \mathrm{d}^3\vec{r}\ |\psi_n|^2
\end{aligned}$$

Therefore, the mean value is equal to an imaginary number times an integral that will be real, so the final answer is, indeed, purely imaginary. □

c) Demonstrate that the above relation remains true if you compute the mean value of the commutator for an arbitrary wave function

$$\Psi = \sum_n c_n \psi_n$$

Hint: Organize the total sum that you obtain in pairs that share the same values of m and n, and demonstrate that when you add up the two terms with the same values of m and n, you obtain a purely imaginary number. The terms in the total sum for which $m = n$ don't have pairs, but you can use the result of part (b) to show that they are indeed imaginary.

Answer. We are interested in computing

$$\langle\Psi|[\hat{O}_1, \hat{O}_2]|\Psi\rangle$$

Taking the hint, we break it into two sums as follows.

$$\begin{aligned}
\langle\Psi|[\hat{O}_1, \hat{O}_2]|\Psi\rangle &= \left\langle \sum_n c_n\psi_n \middle| [\hat{O}_1, \hat{O}_2] \middle| \sum_n c_n\psi_n \right\rangle \\
&= \sum_{n,m} \langle c_n\psi_n|[\hat{O}_1, \hat{O}_2]|c_m\psi_m\rangle \\
&= \sum_m \sum_{\substack{n \\ n=m}} c_n^* c_n \langle\psi_n|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle + \sum_m \sum_{\substack{n \\ n\neq m}} c_m^* c_n \langle\psi_m|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle \\
&= \sum_n c_n^* c_n \langle\psi_n|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle \\
&\quad + \sum_{m<n} (c_m^* c_n \langle\psi_m|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle + c_n^* c_m \langle\psi_n|[\hat{O}_1, \hat{O}_2]|\psi_m\rangle) \\
&= \sum_n c_n^* c_n \langle\psi_n|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle \\
&\quad + \sum_{m<n} [c_m^* c_n \langle\psi_m|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle - c_n^* c_m (\langle\psi_m|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle)^*] \\
&= \sum_n c_n^* c_n \langle\psi_n|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle \\
&\quad + \sum_{m<n} [c_m^* c_n \langle\psi_m|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle - (c_m^* c_n \langle\psi_m|[\hat{O}_1, \hat{O}_2]|\psi_n\rangle)^*]
\end{aligned}$$

From part (b), the first sum is a sum of purely imaginary numbers. Additionally, by the same logic as in part (b), the second sum is a sum of purely imaginary numbers. Thus, the overall term is a sum of purely imaginary numbers, and is thus a purely imaginary number, as desired[1]. □

[1]Note that in the above derivation, I derive that terms across the diagonal from each other are complex conjugates of each other. However, I don't even need to do this because the commutator is Hermitian, so we have this by definition!

2 Infinite Well Motion and Quantum Tunneling

1/19: **1.** In class, we demonstrated that given a certain time-independent potential, one can find solutions to the Schrödinger equation such that

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi_n(\vec{r}) + V(\vec{r})\psi_n(\vec{r}) = E_n\psi_n(\vec{r}) \tag{2.1}$$

Assume now that we are in one dimension, with the potential being a square well:

$$\begin{aligned} &V(x) \to \infty \quad \text{for } x \le 0 \text{ and } x \ge a \\ &V(x) \to 0 \quad\ \ \text{for } 0 < x < a \end{aligned} \tag{2.2}$$

Show that in such a case, the solutions are given by

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \tag{2.3}$$

due to the fact that in order to get a finite mean energy value, the wave function must vanish at $x = 0, a$. The energy eigenstates are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2.4}$$

The factor $\sqrt{2/a}$ comes from the requirement of a good normalized solution, i.e., one with $\langle\psi_n|\psi_n\rangle = 1$. Now, imagine that at $t = 0$, the particle is in the state

$$\psi(x,0) = \frac{A}{\sqrt{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right) \tag{2.5}$$

where A is a real constant.

a) Find the value of A such that $\psi(x,0)$ is normalized. (Hint: Use $\langle\psi_n|\psi_m\rangle = \delta_{nm}$.)

Answer. For $\psi(x,0)$ to be normalized, it must satisfy

$$\langle\psi(x,0)|\psi(x,0)\rangle = 1$$

Now recognize that $\psi(x,0)$ is of the form

$$\psi = c_1\psi_1 + c_3\psi_3 + c_5\psi_5$$

Thus, we have that

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle \\ &= \langle c_1\psi_1 + c_3\psi_3 + c_5\psi_5|c_1\psi_1 + c_3\psi_3 + c_5\psi_5\rangle \\ &= \langle c_1\psi_1|c_1\psi_1\rangle + \langle c_3\psi_3|c_3\psi_3\rangle + \langle c_5\psi_5|c_5\psi_5\rangle + 2\underbrace{\langle c_1\psi_1|c_3\psi_3\rangle}_{0} + 2\underbrace{\langle c_1\psi_1|c_5\psi_5\rangle}_{0} + 2\underbrace{\langle c_3\psi_3|c_5\psi_5\rangle}_{0} \\ &= \langle c_1\psi_1|c_1\psi_1\rangle + \langle c_3\psi_3|c_3\psi_3\rangle + \langle c_5\psi_5|c_5\psi_5\rangle \\ &= \int_0^a \frac{A^2}{a}\sin^2\left(\frac{\pi x}{a}\right)\mathrm{d}x + \int_0^a \frac{3}{5a}\sin^2\left(\frac{3\pi x}{a}\right)\mathrm{d}x + \int_0^a \frac{1}{5a}\sin^2\left(\frac{5\pi x}{a}\right)\mathrm{d}x \\ &= \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} \\ &= \frac{5A^2+4}{10} \end{aligned}$$

$$\boxed{A = \sqrt{\frac{6}{5}}}$$

$\square$

b) If measurements of the energy are carried out, what are the values that will be found and what are the probabilities of measuring such energies? Calculate the average energy.

Answer. As mentioned above, $\psi(x,0)$ is of the form

$$\psi(x,0) = c_1\psi_1(x) + c_3\psi_3(x) + c_5\psi_5(x)$$

Thus, the energies that will be found are

$$\boxed{E_1 = \frac{\hbar^2\pi^2}{2ma^2} \qquad E_3 = \frac{3^2\hbar^2\pi^2}{2ma^2} \qquad E_5 = \frac{5^2\hbar^2\pi^2}{2ma^2}}$$

Moreover, the probabilities of measuring such energies are given by the integrals calculated in part (a). In other words, the probabilities P_i of measuring energy E_i are

$$\boxed{P_1 = \frac{6}{10} \qquad P_3 = \frac{3}{10} \qquad P_5 = \frac{1}{10}}$$

The average energy could be calculated by evaluating $\langle\psi|\hat{H}|\psi\rangle$, or by calculating

$$\langle E\rangle = E_1P_1 + E_3P_3 + E_5P_5$$
$$\boxed{\langle E\rangle = \frac{29\hbar^2\pi^2}{10ma^2}}$$

□

c) Find the expression of the wave function at a later time t. (Hint: What is $\psi_n(x,t)$?)

Answer. Taking the hint, we know that

$$\psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_nt/\hbar} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\mathrm{e}^{-iE_nt/\hbar}$$

We can rewrite $\psi(x,0)$ in a form relatable to the above as follows.

$$\begin{aligned}\psi(x,0) &= \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)\\ &= \sqrt{\frac{3}{5}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)\\ &= \sqrt{\frac{3}{5}}\psi_1(x,0) + \sqrt{\frac{3}{10}}\psi_3(x,0) + \frac{1}{\sqrt{10}}\psi_5(x,0)\end{aligned}$$

Therefore,

$$\begin{aligned}\psi(x,t) &= \sqrt{\frac{3}{5}}\psi_1(x,t) + \sqrt{\frac{3}{10}}\psi_3(x,t) + \frac{1}{\sqrt{10}}\psi_5(x,t)\\ &= \sqrt{\frac{3}{5}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\mathrm{e}^{-iE_1t/\hbar} + \sqrt{\frac{3}{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{3\pi x}{a}\right)\mathrm{e}^{-iE_3t/\hbar}\\ &\quad + \frac{1}{\sqrt{10}}\sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)\mathrm{e}^{-iE_5t/\hbar}\end{aligned}$$

$$\boxed{\psi(x,t) = \sqrt{\frac{6}{5a}}\sin\left(\frac{\pi x}{a}\right)\mathrm{e}^{-iE_1t/\hbar} + \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right)\mathrm{e}^{-iE_3t/\hbar} + \frac{1}{\sqrt{5a}}\sin\left(\frac{5\pi x}{a}\right)\mathrm{e}^{-iE_5t/\hbar}}$$

□

d) Is the mean value of the position operator independent of time? What about the mean value of the momentum? (Hint: Use symmetry properties with respect to the central point of the well.)

Answer. To determine whether or not the position operator is independent of time, it will suffice to evaluate

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\langle\psi(x,t)|\hat{\vec{x}}|\psi(x,t)\rangle\Big)$$

If the above expression is equal to zero, then the position operator is independent of time, and if it is not equal to zero, then the position operator is not independent of time. Let's begin.
We have that

$$\begin{aligned}
&\langle\psi(x,t)|\hat{\vec{x}}|\psi(x,t)\rangle\\
&=\left\langle\frac{3}{5}\psi_1\mathrm{e}^{-iE_1t/\hbar}+\frac{3}{10}\psi_3\mathrm{e}^{-iE_3t/\hbar}+\frac{1}{10}\psi_5\mathrm{e}^{-iE_5t/\hbar}\middle|\hat{\vec{x}}\middle|\frac{3}{5}\psi_1\mathrm{e}^{-iE_1t/\hbar}+\frac{3}{10}\psi_3\mathrm{e}^{-iE_3t/\hbar}+\frac{1}{10}\psi_5\mathrm{e}^{-iE_5t/\hbar}\right\rangle\\
&=\frac{9}{25}\mathrm{e}^{-2iE_1t/\hbar}\langle\psi_1|\hat{\vec{x}}|\psi_1\rangle+\frac{9}{100}\mathrm{e}^{-2iE_3t/\hbar}\langle\psi_3|\hat{\vec{x}}|\psi_3\rangle+\frac{1}{100}\mathrm{e}^{-2iE_5t/\hbar}\langle\psi_5|\hat{\vec{x}}|\psi_5\rangle\\
&\quad+\frac{9}{50}\mathrm{e}^{-i(E_1+E_3)t/\hbar}\langle\psi_1|\hat{\vec{x}}|\psi_3\rangle+\frac{3}{50}\mathrm{e}^{-i(E_1+E_5)t/\hbar}\langle\psi_1|\hat{\vec{x}}|\psi_5\rangle+\frac{3}{100}\mathrm{e}^{-i(E_3+E_5)t/\hbar}\langle\psi_3|\hat{\vec{x}}|\psi_5\rangle
\end{aligned}$$

Now, computing integrals, we have the following.

$$\langle\psi_1|\hat{\vec{x}}|\psi_3\rangle=\langle\psi_1|\hat{\vec{x}}|\psi_5\rangle=\langle\psi_3|\hat{\vec{x}}|\psi_5\rangle=0$$

One easy way to see this without direct computation is to observe, per the hint, that $(x-0.5a)\psi_1\psi_3$ and $0.5a\psi_1\psi_3$ are both odd about the central point of the well and hence evaluate to zero. Thus,

$$\langle\psi_1|\hat{\vec{x}}|\psi_3\rangle=\int_0^a x\psi_1\psi_3\,\mathrm{d}x=\int_0^a(x-0.5a)\psi_1\psi_3\,\mathrm{d}x+\int_0^a 0.5a\psi_1\psi_3\,\mathrm{d}x=0+0=0$$

On the other hand, we may observe that $x\psi_i^2$ $(i=1,3,5)$ are all strictly positive on $(0,a)$ and hence evaluate to positive constants c_i. Consequently,

$$\langle\psi(x,t)|\hat{\vec{x}}|\psi(x,t)\rangle=\frac{9}{25}c_1\mathrm{e}^{-2iE_1t/\hbar}+\frac{9}{100}c_3\mathrm{e}^{-2iE_3t/\hbar}+\frac{1}{100}c_5\mathrm{e}^{-2iE_5t/\hbar}$$

This function clearly has a nonzero derivative with respect to time, meaning that the mean value of the position operator $\boxed{\text{is not}}$ independent of time.
As to the second part of the question, we have that

$$\frac{\mathrm{d}\langle\hat{\vec{p}}\rangle}{\mathrm{d}t}=\frac{\mathrm{d}}{\mathrm{d}t}\left(m\frac{\mathrm{d}\langle\hat{\vec{x}}\rangle}{\mathrm{d}t}\right)\neq0$$

Therefore, the mean value of the momentum operator $\boxed{\text{is not}}$ independent of time, either. □

e) Would the result of part (d) be different if we replaced ψ_3 by ψ_2 in Eq. 2.5?

Answer. If we replaced ψ_3 by ψ_2, then we would additionally have

$$\langle\psi_1|\hat{\vec{x}}|\psi_2\rangle\neq0\qquad\qquad\langle\psi_2|\hat{\vec{x}}|\psi_5\rangle\neq0$$

However, $\boxed{\text{this would change neither result overall.}}$ □

2. a) Consider now the wave function $\Psi(x,t)$ of a particle moving in one dimension in a potential $V(x)$ such that

$$\begin{aligned} V(x) &\to \infty && \text{for } |x| \geq a/2 \\ V(x) &= 0 && \text{for } -a/2 < x < 0 \\ V(x) &= V_0 && \text{for } 0 \leq x < a/2 \end{aligned} \tag{2.6}$$

Considering that the wave function and its derivative are continuous at $x = 0$, and that the wave function vanishes at $x = \pm a/2$, try to find the equation that gives the possible energy states assuming $E_n > V_0$.

Hint: There are different combinations of sine and cosine functions for positive and negative values of x.

Answer. Taking the hint, split the total wave function $\psi(x)$ into the sum of two parts, $\psi_1(x)$ and $\psi_2(x)$, where $\psi_1(x) = 0$ for $x \geq 0$ and $\psi_2(x) = 0$ for $x \leq 0$. In general, we have

$$\psi_1(x) = A\sin(kx) + B\cos(kx) \qquad \psi_2(x) = C\sin(k_2 x) + D\cos(k_2 x)$$

If $\psi = \psi_1 + \psi_2$ is to be continuous at $x = 0$, then we must have

$$\begin{gathered} \psi_1(0) = \psi_2(0) \\ B = D \end{gathered}$$

If $\psi = \psi_1 + \psi_2$ is to have a continuous first derivative at $x = 0$, then we must have

$$\begin{gathered} \psi_1'(0) = \psi_2'(0) \\ kA = k_2 C \end{gathered}$$

Thus, altogether, we have that

$$\psi(x) = \begin{cases} A\sin(kx) + B\cos(kx) & x \leq 0 \\ \frac{kA}{k_2}\sin(k_2 x) + B\cos(k_2 x) & x > 0 \end{cases} \qquad \text{for } |x| \leq a/2$$

The boundary condition is met when either...

i. $B = 0$, $k = n\pi$, and $k_2 = m\pi/a$;

ii. $A = 0$, $k = n\pi/2$, and $k_2 = m\pi/2a$.

$\square$

3 The Harmonic Oscillator

1/26: **1.** Harmonic oscillator in Earth's gravity.

In class, we solved the Harmonic Oscillator Problem, which has the potential

$$V(x) = \frac{m\omega^2 x^2}{2} \tag{3.1}$$

with $\omega = \sqrt{k/m}$ being the classical frequency. Now assume that x is a vertical direction and that we place the harmonic oscillator close to the Earth's surface. Now, if x grows upwards, the potential will be

$$V(x) = \frac{m\omega^2 x^2}{2} + mgx + C \tag{3.2}$$

with $g = 9.8\,\mathrm{m/s^2}$ and C an arbitrary (and irrelevant) constant.

a) First, think about the classical problem. The equilibrium point is no longer at $x = 0$, but a displaced point where the tension and gravity forces are equilibrated. Find that point and rewrite the potential in terms of a new variable representing departures from the equilibrium point. What would be the motion of a classical particle under the potential given in Eq. 3.2?

Answer. The equilibrium point x_{eq} will correspond to a minimum of V. Thus, we may solve

$$V'(x_{\text{eq}}) = 0$$

for x_{eq}. Doing this, we obtain

$$\begin{aligned}
0 &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{m\omega^2 x^2}{2} + mgx + C\right)\Bigg|_{x_{\text{eq}}} \\
&= m\omega^2 x_{\text{eq}} + mg \\
&\boxed{x_{\text{eq}} = -\frac{g}{\omega^2}}
\end{aligned}$$

Let

$$u := x - x_{\text{eq}}$$

Then $x = u + x_{\text{eq}}$, so

$$\begin{aligned}
V(u) &= \frac{m\omega^2 (u + x_{\text{eq}})^2}{2} + mg(u + x_{\text{eq}}) + C \\
&= \frac{m\omega^2 u^2}{2} + m\omega^2 x_{\text{eq}} u + mgu + \frac{m\omega^2 x_{\text{eq}}^2}{2} + mgx_{\text{eq}} + C \\
V(u) &= \frac{m\omega^2 u^2}{2} + m\omega^2\left(-\frac{g}{\omega^2}\right)u + mgu + C \\
&\boxed{V(u) = \frac{m\omega^2 u^2}{2} + C}
\end{aligned}$$

Note that we combine all constants from the second to the third line above, which we may do because only relative — not absolute — values of the potential matter.

This result reveals that the motion of a classical particle under the potential given in Eq. 3.2 is $\boxed{\text{simple harmonic motion about } x_{\text{eq}}.}$ □

b) Now think about the quantum problem. Without gravity, the energy eigenvalues are given by $E_n^{\text{HO}} = \hbar\omega(n+1/2)$ and the corresponding wave functions ψ_n^{HO} can be written in terms of odd and even Hermite polynomials and a Gaussian function of x. (Here, HO means "harmonic oscillator.") Using these results, derive the new energy eigenvalues E_n and eigenfunctions ψ_n in the presence of gravity, Eq. 3.2. *Hint*: Can you make a similar redefinition of the coordinates as you did in the classical case?

Answer. To derive E_n, ψ_n, we must solve the following ODE.

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) + \left[\frac{m\omega^2 x^2}{2} + mgx + C\right]\psi_n(x) = E_n\psi_n(x)$$

Define u as in part (a). Fold C into the energy to get rid of it, and substitute $\psi_n(u)$ and $x = u + x_{\text{eq}}$ into the above equation.

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}x}\psi_n(u)\right] + \frac{m\omega^2 u^2}{2}\psi_n(u) = E_n\psi_n(u)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\mathrm{d}}{\mathrm{d}u}\psi_n(u)\cdot\underbrace{\frac{\mathrm{d}u}{\mathrm{d}x}}_{1}\right] + \frac{m\omega^2 u^2}{2}\psi_n(u) = E_n\psi_n(u)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}u}\left[\frac{\mathrm{d}}{\mathrm{d}u}\psi_n(u)\right]\cdot\underbrace{\frac{\mathrm{d}u}{\mathrm{d}x}}_{1} + \frac{m\omega^2 u^2}{2}\psi_n(u) = E_n\psi_n(u)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}u^2}\psi_n(u) + \frac{m\omega^2 u^2}{2}\psi_n(u) = E_n\psi_n(u)$$

We worked out the solutions to this equation already in class. They are

$$\psi_n(u) = \psi_n^{\text{HO}}(u) \qquad\qquad E_n = E_n^{\text{HO}}$$

It follows by returning the substitution that

$$\boxed{\psi_n(x) = \psi_n^{\text{HO}}(x - x_{\text{eq}})} \qquad\qquad \boxed{E_n = E_n^{\text{HO}}}$$

□

c) What would be the mean value of x and p in this system (for a given energy eigenstate, not a generic state)? What would be the mean value of x^2 and p^2 in the ground state of the system? *Hint*: Use properties of the wave functions under displacements from the equilibrium point, and write $x = x_{\text{eq}} + (x - x_{\text{eq}})$, where x_{eq} is the equilibrium point.

Answer. Piggybacking off of the results from class, we will have

$$\boxed{\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle = x_{\text{eq}}} \qquad\qquad \boxed{\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle = 0}$$

□

d) Think about the uncertainty principle. What is the value of $\sigma_x\sigma_p$ in the ground state of this system? Does it differ from the value we obtained in the absence of gravity?

2. Bouncing harmonic oscillator.

Assume now that we add an infinite potential floor just at the equilibrium point, so that the particle can no longer go below it. Under this modification, the new potential is

$$V(x) = \begin{cases} \frac{m\omega^2 x^2}{2} + mgx + C & x > x_{\text{eq}} \\ \infty & x \leq x_{\text{eq}} \end{cases} \tag{3.3}$$

where x_{eq} is the equilibrium point. Classically, every time the particle hits the floor, it will bounce back with the same modulus of the momentum, but in the upwards direction.

a) What is the mathematical description of $x(t)$ of the classical motion? *Hint*: Think about the oscillator without a floor and the symmetry regarding displacements in the positive and negative directions from the equilibrium point.

b) Now go back to the quantum mechanical problem. Similarly to the infinite square well that we solved last week, what should happen to the wave functions at $x = x_{\text{eq}}$ and why?

c) Now look at the Schrödinger equation for positive values of the displacement with respect to the equilibrium point. Does it change from the one we had without the floor? Find the energy eigenvalues and the corresponding functions ψ_n to this problem. *Hint*: Observe that the boundary condition at $x = x_{\text{eq}}$ eliminates some solutions.

d) What is the minimal energy solution once we add the floor to the system? Is it the same as the system without the floor? What is the corresponding eigenfunction of this solution?

e) Find σ_x and σ_p for the minimum energy solution. Is $\sigma_x\sigma_p$ the same as in the system without the wall?

3. For the harmonic oscillator, consider the ladder operators $a_\pm = (\mp ip + m\omega x)/\sqrt{2\hbar m\omega}$. Recall that $[a_-, a_+] = 1$, the Hamiltonian may be written as $\hat{H} = \hbar\omega(a_+a_- + 1/2)$, and the eigenfunctions describing the eigenstates of energy $E_n = \hbar\omega(n + 1/2)$ are related by $a_+\psi_n = \sqrt{n+1}\psi_{n+1}$ and $a_-\psi_n = \sqrt{n}\psi_{n-1}$.

a) Compute the mean value of x and p in the energy eigenstates described by ψ_n.

Answer. We have that

$$\begin{aligned}\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left[\langle\psi_n|a_+|\psi_n\rangle + \langle\psi_n|a_-|\psi_n\rangle\right] \\ &= \sqrt{\frac{\hbar}{2m\omega}}\Big[\sqrt{n+1}\underbrace{\langle\psi_n|\psi_{n+1}\rangle}_{0} + \sqrt{n}\underbrace{\langle\psi_n|\psi_{n-1}\rangle}_{0}\Big]\end{aligned}$$

$$\boxed{\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle = 0}$$

and

$$\begin{aligned}\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle &= i\sqrt{\frac{\hbar m\omega}{2}}\left[\langle\psi_n|a_+|\psi_n\rangle - \langle\psi_n|a_-|\psi_n\rangle\right] \\ &= i\sqrt{\frac{\hbar m\omega}{2}}\Big[\sqrt{n+1}\underbrace{\langle\psi_n|\psi_{n+1}\rangle}_{0} - \sqrt{n}\underbrace{\langle\psi_n|\psi_{n-1}\rangle}_{0}\Big]\end{aligned}$$

$$\boxed{\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle = 0}$$

□

b) Compute the mean value of x^2 and p^2 in these states.

Answer. As derived in class, we have that

$$\left\langle\psi_n\middle|\frac{k\hat{\vec{x}}^2}{2}\middle|\psi_n\right\rangle = \frac{E_n}{2} \qquad \left\langle\psi_n\middle|\frac{\hat{\vec{p}}^2}{2m}\middle|\psi_n\right\rangle = \frac{E_n}{2}$$

Therefore,

$$\langle\psi_n|\hat{\vec{x}}^2|\psi_n\rangle = \frac{2}{k}\cdot\frac{E_n}{2} \qquad \langle\psi_n|\hat{\vec{p}}^2|\psi_n\rangle = 2m\cdot\frac{E_n}{2}$$

$$\boxed{\langle\psi_n|\hat{\vec{x}}^2|\psi_n\rangle = \frac{\hbar\omega}{k}\left(n+\frac{1}{2}\right)} \qquad \boxed{\langle\psi_n|\hat{\vec{p}}^2|\psi_n\rangle = \hbar\omega m\left(n+\frac{1}{2}\right)}$$

□

c) What would the uncertainty principle tell me about $\sigma_x\sigma_p$?

Answer. Since

$$\sigma_x^2 = \langle\psi_n|\hat{\vec{x}}^2|\psi_n\rangle - (\langle\psi_n|\hat{\vec{x}}|\psi_n\rangle)^2 \qquad\qquad \sigma_p^2 = \langle\psi_n|\hat{\vec{p}}^2|\psi_n\rangle - (\langle\psi_n|\hat{\vec{p}}|\psi_n\rangle)^2$$

we have that

$$\sigma_x^2 \cdot \sigma_p^2 = \hbar^2\left(n+\frac{1}{2}\right)^2$$

$$\boxed{\sigma_x\sigma_p = \frac{\hbar}{2}(2n+1)}$$

□

d) Verify that the uncertainty principle is fulfilled for the energy eigenstates.

Answer. Per part (c), we have that

$$\sigma_x\sigma_p = \frac{\hbar}{2}(2n+1) \geq \frac{\hbar}{2}$$

for all $n \geq 0$, as desired. □

e) Write a formal expression for the mean value of the position and the momentum for the general solution $\psi(x,t)$. Work it out as much as you can, using the orthonormality of the wave functions ψ_n.
Hint: For instance, the mean value of the operators x^q and p^q can be obtained by computing

$$\langle x^q\rangle = \left(\frac{\hbar}{2m\omega}\right)^{q/2}\int \psi(x)^*(a_+ + a_-)^q\psi(x)\,\mathrm{d}x \tag{3.4}$$

and

$$\langle p^q\rangle = i^q\left(\frac{\hbar}{2m\omega}\right)^{q/2}\int \psi(x)^*(a_+ - a_-)^q\psi(x)\,\mathrm{d}x \tag{3.5}$$

Observe that due to orthonormality of the real functions ψ_n and the fact that $a_\pm$ are ladder operators, the only nonvanishing contributions are

$$\begin{aligned}
\int \psi_m(x)a_+^q\psi_n(x)\,\mathrm{d}x &\qquad \text{Non-vanishing for } m = n+q\\
\int \psi_m(x)a_-^q\psi_n(x)\,\mathrm{d}x &\qquad \text{Non-vanishing for } m = n-q\\
\int \psi_m(x)a_-^q a_+^r\psi_n(x)\,\mathrm{d}x &\qquad \text{Non-vanishing for } m = n+r-q\\
\int \psi_m(x)a_+^q a_-^r\psi_n(x)\,\mathrm{d}x &\qquad \text{Non-vanishing for } m = n-r+q
\end{aligned} \tag{3.6}$$

Two useful cases, as follows from the above, are $\langle\psi_n|a_+a_-|\psi_n\rangle = n$ and $\langle\psi_n|a_-a_+|\psi_n\rangle = n+1$.

4 Observables and Operators

2/3: **1.** Imagine a one-dimensional free particle ($V(x) = 0$) of mass m whose mean value of the position and momentum at time $t = 0$ are given by x_0 and p_0.

a) Demonstrate that the mean value of the momentum and its powers is time-independent, that is

$$\frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{p}^n|\psi\rangle) = 0 \tag{4.1}$$

Hint: Use the fact that for time-independent operators, $\mathrm{d}\langle\psi|\hat{O}|\psi\rangle\big/\mathrm{d}t = (i/\hbar)\langle\psi|[\hat{H},\hat{O}]|\psi\rangle$.

Answer. To prove that the mean value of the momentum is time-independent, it will suffice to show that

$$[\hat{H},\hat{p}^n] = 0$$

for all $n \in \mathbb{N}$. To do so, we induct on n. For the base case $n = 1$, we have that

$$[\hat{H},\hat{p}] = \left[\frac{\hat{p}^2}{2m},\hat{p}\right] = \frac{1}{2m}(\hat{p}^3 - \hat{p}^3) = 0$$

Now suppose inductively that we have prove the claim for n, that is, we know that $[\hat{H},\hat{p}^n] = 0$; we now seek to prove the claim for $n + 1$. Here, we have that

$$[\hat{H},\hat{p}^{n+1}] = \hat{p}\underbrace{[\hat{H},\hat{p}^n]}_{0} + \underbrace{[\hat{H},\hat{p}^n]}_{0}\hat{p} = 0$$

This closes the induction. □

b) Compute $\mathrm{d}\langle\psi|\hat{x}|\psi\rangle/\mathrm{d}t$, and show that

$$\langle\psi|\hat{x}|\psi\rangle(t) = \frac{p_0 t}{m} + x_0 \tag{4.2}$$

Answer. We have from Lecture 1.2 that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{x}|\psi\rangle) = \frac{\langle\psi|\hat{p}|\psi\rangle}{m}$$

Now part (a) tells us that $\langle\psi|\hat{p}|\psi\rangle$ is time-independent, which means that if $\langle\psi|\hat{p}|\psi\rangle = p_0$ at $t = 0$, then $\langle\psi|\hat{p}|\psi\rangle = p_0$ for all time t. Thus,

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{x}|\psi\rangle) = \frac{p_0}{m}}$$

It follows by integrating that

$$\begin{aligned}
\int_0^t \frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{x}|\psi\rangle)\,\mathrm{d}t &= \int_0^t \frac{p_0}{m}\,\mathrm{d}t' \\
\langle\psi|\hat{x}|\psi\rangle(t) - \langle\psi|\hat{x}|\psi\rangle(0) &= \frac{p_0}{m}t - \frac{p_0}{m}0 \\
\langle\psi|\hat{x}|\psi\rangle(t) - x_0 &= \frac{p_0 t}{m} \\
\langle\psi|\hat{x}|\psi\rangle(t) &= \frac{p_0 t}{m} + x_0
\end{aligned}$$

as desired. □

c) Show also that

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(\langle\psi|\hat{x}^2|\psi\rangle\big) = \frac{2}{m}\langle\psi|\hat{p}\hat{x}|\psi\rangle + \frac{i\hbar}{m} \tag{4.3}$$

Hint: Use the fact that $[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$ and $[\hat{A},\hat{B}\hat{C}] = \hat{B}[\hat{A},\hat{C}] + [\hat{A},\hat{B}]\hat{C}$.

Answer. We have that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\big(\langle\psi|\hat{x}^2|\psi\rangle\big) &= \frac{i}{\hbar}\langle\psi|[\hat{H},\hat{x}^2]|\psi\rangle \\
&= \frac{i}{2m\hbar}\langle\psi|[\hat{p}^2,\hat{x}^2]|\psi\rangle \\
&= \frac{i}{2m\hbar}\langle\psi|\hat{p}[\hat{p},\hat{x}^2] + [\hat{p},\hat{x}^2]\hat{p}|\psi\rangle \\
&= \frac{i}{2m\hbar}\langle\psi|\hat{p}(\hat{x}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{x}) + (\hat{x}[\hat{p},\hat{x}] + [\hat{p},\hat{x}]\hat{x})\hat{p}|\psi\rangle \\
&= \frac{i}{2m\hbar}\big(\langle\psi|\hat{p}\hat{x}[\hat{p},\hat{x}]|\psi\rangle + \langle\psi|\hat{p}[\hat{p},\hat{x}]\hat{x}|\psi\rangle + \langle\psi|\hat{x}[\hat{p},\hat{x}]\hat{p}|\psi\rangle + \langle\psi|[\hat{p},\hat{x}]\hat{x}\hat{p}|\psi\rangle\big) \\
&= \frac{i}{2m\hbar}\big(\langle\psi|\hat{p}\hat{x}(-i\hbar)|\psi\rangle + \langle\psi|\hat{p}(-i\hbar)\hat{x}|\psi\rangle + \langle\psi|\hat{x}(-i\hbar)\hat{p}|\psi\rangle + \langle\psi|(-i\hbar)\hat{x}\hat{p}|\psi\rangle\big) \\
&= \frac{1}{2m}\big(\langle\psi|\hat{p}\hat{x}|\psi\rangle + \langle\psi|\hat{p}\hat{x}|\psi\rangle + \langle\psi|\hat{x}\hat{p}|\psi\rangle + \langle\psi|\hat{x}\hat{p}|\psi\rangle\big) \\
&= \frac{1}{2m}(2\langle\psi|\hat{p}\hat{x}|\psi\rangle + 2\langle\psi|\hat{p}\hat{x} + i\hbar|\psi\rangle) \\
&= \frac{1}{2m}(4\langle\psi|\hat{p}\hat{x}|\psi\rangle + 2i\hbar\langle\psi|\psi\rangle) \\
&= \frac{2}{m}\langle\psi|\hat{p}\hat{x}|\psi\rangle + \frac{i\hbar}{m}
\end{aligned}$$

as desired. □

d) Compute, in terms of $\langle\psi|\hat{p}^2|\psi\rangle$ and $\langle\psi|\hat{p}|\psi\rangle$, the values of

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\big(\langle\psi|\hat{x}^2|\psi\rangle\big) \qquad\qquad \frac{\mathrm{d}^2}{\mathrm{d}t^2}\big[(\langle\psi|\hat{x}|\psi\rangle)^2\big] \tag{4.4}$$

Hint: Use the commutation of $\hat{p}\hat{x}$ with $\hat{H} = \hat{p}^2/2m$.

Answer. By part (c), we have that

$$\begin{aligned}
\frac{\mathrm{d}^2}{\mathrm{d}t^2}\big(\langle\psi|\hat{x}^2|\psi\rangle\big) &= \frac{2}{m}\frac{\mathrm{d}}{\mathrm{d}t}\big(\langle\psi|\hat{p}\hat{x}|\psi\rangle\big) \\
&= \frac{2i}{m\hbar}\langle\psi|[\hat{H},\hat{p}\hat{x}]|\psi\rangle \\
&= \frac{i}{m^2\hbar}\Big(\langle\psi|\hat{p}^2\underbrace{[\hat{p},\hat{x}]}_{-i\hbar}|\psi\rangle + \langle\psi|\hat{p}\underbrace{[\hat{p},\hat{p}]}_{0}\hat{x}|\psi\rangle + \langle\psi|\hat{p}\underbrace{[\hat{p},\hat{x}]}_{-i\hbar}\hat{p}|\psi\rangle + \langle\psi|\underbrace{[\hat{p},\hat{p}]}_{0}\hat{x}\hat{p}|\psi\rangle\Big)
\end{aligned}$$

$$\boxed{\frac{\mathrm{d}^2}{\mathrm{d}t^2}\big(\langle\psi|\hat{x}^2|\psi\rangle\big) = \frac{2}{m^2}\langle\psi|\hat{p}^2|\psi\rangle}$$

By part (b), we have that

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left[(\langle\psi|\hat{x}|\psi\rangle)^2\right] &= \frac{\mathrm{d}}{\mathrm{d}t}[2\langle\psi|\hat{x}|\psi\rangle\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{x}|\psi\rangle)] \\ &= 2\frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{x}|\psi\rangle)\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\langle\psi|\hat{x}|\psi\rangle) + 2\langle\psi|\hat{x}|\psi\rangle\cdot\frac{\mathrm{d}^2}{\mathrm{d}t^2}(\langle\psi|\hat{x}|\psi\rangle) \\ &= \frac{2p_0^2}{m^2} + 2x_0\cdot\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{p_0}{m}\right)}_{0}\end{aligned}$$

$$\boxed{\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left[(\langle\psi|\hat{x}|\psi\rangle)^2\right] = \frac{2}{m^2}(\langle\psi|\hat{p}|\psi\rangle)^2}$$

□

e) Show that the position and momentum fluctuations are related by

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}(\sigma_x^2) = \frac{2\sigma_p^2}{m^2} \tag{4.5}$$

where $\sigma_{\hat{O}}^2 = \langle\psi|\hat{O}^2|\psi\rangle - (\langle\psi|\hat{O}|\psi\rangle)^2$, and that the solution to this equation at sufficiently large values of t is given by

$$\sigma_x \approx \frac{\sigma_p t}{m} \tag{4.6}$$

where σ_p is independent of time. Discuss the implications of this result. Can you understand this result intuitively in terms of the fact that the momentum is not well-defined, meaning that there is a probability of finding the particle at different momentum values at a given time?

Answer. By part (d), we have that

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}(\sigma_x^2) &= \frac{\mathrm{d}^2}{\mathrm{d}t^2}(\langle\psi|\hat{x}^2|\psi\rangle) - \frac{\mathrm{d}^2}{\mathrm{d}t^2}\left[(\langle\psi|\hat{x}|\psi\rangle)^2\right] \\ &= \frac{2}{m^2}\left[\langle\psi|\hat{p}^2|\psi\rangle - (\langle\psi|\hat{p}|\psi\rangle)^2\right] \\ &= \frac{2\sigma_p^2}{m^2}\end{aligned}$$

Additionally, we have that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\left[\left(\frac{\sigma_p t}{m}\right)^2\right] = \frac{\mathrm{d}^2}{\mathrm{d}t^2}\left(\frac{\sigma_p^2 t^2}{m^2}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{2\sigma_p^2 t}{m^2}\right) = \frac{2\sigma_p^2}{m^2}$$

Note that by requiring t be "sufficiently large," we are eliminating consideration of the case $t = 0$, in which we would have $\sigma_x = 0$ which cannot happen by the Heisenberg uncertainty principle.

We now discuss the implications of this result. In part (a), we proved that the $\langle\psi|\hat{p}^n|\psi\rangle$ are fixed for all time, which means in particular that

$$\sigma_p^2 = \langle\psi|\hat{p}^2|\psi\rangle - (\langle\psi|\hat{p}|\psi\rangle)^2$$

is fixed. Thus, Eq. 4.6 essentially implies that for sufficiently large time t, the uncertainty in the position of the free particle increases approximately linearly with time. We may visualize this as the particle "spreading out" as time passes, much like a wave function might expand after it collapses.

The fact that the momentum is not well-defined is the *reason* that the particle spreads out over time. Essentially, different "parts" of the particle will move with different momenta, so as the free particle "moves," some parts of it will move faster and some will move slower, causing it to spread out! This further justifies the linear relation, which in these terms essentially says that the greater the uncertainty in momenta, the greater the difference in speed of different parts of the particle, and the greater the spread in x as time goes on. □

2. The power of completeness. Imagine that I have a complete set $\{\psi_n\}$ of energy eigenstate functions and that any given wave function ψ can be expressed as a linear combination of these functions via

$$\psi(x) = \sum_{n=0}^{\infty} c_n \psi_n(x) \tag{4.7}$$

a) Demonstrate, using the fact that $\int \psi_m^*(x)\psi_n(x)\,\mathrm{d}x = \delta_{mn}$, that these functions fulfill a completeness relation, in the sense that

$$\delta(x_1 - x_2) = \sum_m \psi_m(x_1)\psi_m^*(x_2) \tag{4.8}$$

Hint: Demonstrate that if you integrate this sum multiplied by an arbitrary function $\psi(x_2)$, you obtain the same function at the point $\psi(x_1)$.

Answer. Let $\psi : \mathbb{R} \to \mathbb{C}$ be an arbitrary, smooth function in the variable x_2. To prove the equality in Eq. 4.8, it will suffice to show that

$$\int \delta(x_1 - x_2)\psi(x_2)\,\mathrm{d}x_2 = \int \sum_m \psi_m(x_1)\psi_m^*(x_2)\psi(x_2)\,\mathrm{d}x_2$$

Note that this integral and all following integrals are over all space, that is, $(-\infty, \infty)$. By the properties of the Dirac delta function, the left side of the above equality evaluates to

$$\int \delta(x_1 - x_2)\psi(x_2)\,\mathrm{d}x_2 = \psi(x_1)$$

The right side is a bit more complicated since it involves the expansion of ψ that we are allowed to do by Eq. 4.7. However, it evaluates directly all the same, as follows.

$$\begin{aligned}
\int \sum_m \psi_m(x_1)\psi_m^*(x_2)\psi(x_2)\,\mathrm{d}x_2 &= \int \sum_m \psi_m(x_1)\psi_m^*(x_2)\left(\sum_{n=0}^{\infty} c_n\psi_n(x_2)\right)\mathrm{d}x_2 \\
&= \sum_m \sum_{n=0}^{\infty} c_n\psi_m(x_1) \int \psi_m^*(x_2)\psi_n(x_2)\,\mathrm{d}x_2 \\
&= \sum_{n=0}^{\infty} c_n\psi_n(x_1) \\
&= \psi(x_1)
\end{aligned}$$

Therefore, by transitivity, we have the desired equality. □

b) Imagine that you want to calculate the mean value of some real function $h(x)$ of the operator $\hat{x} = x$ that can be expressed as a product of two real functions, i.e., $h(x) = f(x)g(x)$. For instance, $x^4 = x^2x^2$. Then to compute the mean value of $h(x)$ in a particular energy eigenstate described by ψ_n, one needs to compute

$$\langle\psi_n|h(x)|\psi_n\rangle = \int \psi_n^*(x)f(x)g(x)\psi_n(x)\,\mathrm{d}x = \iint \psi_n^*(x_1)f(x_1)\delta(x_1 - x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \tag{4.9}$$

Verify that this is true by performing the integral over one of two variables, x_1 or x_2.

Answer. Working backward from the RHS of Eq. 4.9, we have that

$$\begin{aligned}
\text{RHS} &= \iint \psi_n^*(x_1)f(x_1)\delta(x_1-x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&= \int \left[\int \psi_n^*(x_1)f(x_1)\delta(x_1-x_2)\,\mathrm{d}x_1\right] g(x_2)\psi_n(x_2)\,\mathrm{d}x_2 \\
&= \int \left[\psi_n^*(x_2)f(x_2)\right] g(x_2)\psi_n(x_2)\,\mathrm{d}x_2 \\
&= \int \psi_n^*(x)f(x)g(x)\psi_n(x)\,\mathrm{d}x \\
&= \int \psi_n^*(x)h(x)\psi_n(x)\,\mathrm{d}x \\
&= \langle\psi_n|h(x)|\psi_n\rangle
\end{aligned}$$

□

c) Use this expression to obtain the mean value of $h(x)$ as a function of a sum of the products of the matrix elements $f_{mn}(x)$ and $g_{mn}(x)$, defined as

$$f_{mn} = \int \psi_m^*(x)f(x)\psi_n(x)\,\mathrm{d}x \qquad g_{mn} = \int \psi_m^*(x)g(x)\psi_n(x)\,\mathrm{d}x \tag{4.10}$$

Answer. By part (a) and Eq. 4.8, we have that

$$\begin{aligned}
\langle\psi_n|h(x)|\psi_n\rangle &= \iint \psi_n^*(x_1)f(x_1)\delta(x_1-x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&= \iint \psi_n^*(x_1)f(x_1)\left[\sum_m \psi_m(x_1)\psi_m^*(x_2)\right] g(x_2)\psi_n(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&= \sum_m \iint \psi_n^*(x_1)f(x_1)\psi_m(x_1)\psi_m^*(x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_1\,\mathrm{d}x_2 \\
&= \sum_m \int \left[\int \psi_n^*(x_1)f(x_1)\psi_m(x_1)\,\mathrm{d}x_1\right] \psi_m^*(x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_2 \\
&= \sum_m \int f_{nm}\psi_m^*(x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_2 \\
&= \sum_m f_{nm}\int \psi_m^*(x_2)g(x_2)\psi_n(x_2)\,\mathrm{d}x_2
\end{aligned}$$

$$\boxed{\langle\psi_n|h(x)|\psi_n\rangle = \sum_m f_{nm}g_{mn}}$$

□

d) Apply the above to compute the mean value of $x^4 = x^2x^2$ for the harmonic oscillator in its energy eigenstate. *Hint*: Use the ladder operators.

Answer. By part (b), we have that

$$\begin{aligned}
\langle\psi_n|x^4|\psi_n\rangle &= \sum_m \langle n|x^2|m\rangle\ \langle m|x^2|n\rangle \\
&= \frac{\hbar^2}{4m^2\omega^2}\sum_m \langle n|(a_+ + a_-)^2|m\rangle\ \langle m|(a_+ + a_-)^2|n\rangle \\
&= \frac{\hbar^2}{4m^2\omega^2}\sum_m \Big(\langle n|a_+^2|m\rangle + \langle n|a_-^2|m\rangle + 2\langle n|a_+a_-|m\rangle + \langle n|1|m\rangle\Big) \\
&\quad\cdot\Big(\langle m|a_+^2|n\rangle + \langle m|a_-^2|n\rangle + 2\langle m|a_+a_-|n\rangle + \langle m|1|n\rangle\Big) \\
&= \frac{\hbar^2}{4m^2\omega^2}\sum_m \Big(\sqrt{(m+1)(m+2)}\,\langle n|m+2\rangle + \sqrt{m(m-1)}\,\langle n|m-2\rangle + (2m+1)\,\langle n|m\rangle\Big) \\
&\quad\cdot\Big(\sqrt{(n+1)(n+2)}\,\langle m|n+2\rangle + \sqrt{n(n-1)}\,\langle m|n-2\rangle + (2n+1)\,\langle m|n\rangle\Big) \\
&= \frac{\hbar^2}{4m^2\omega^2}\Big(\sqrt{(n-1)n}\,\langle n|n\rangle + \sqrt{(n+2)(n+1)}\,\langle n|n\rangle + (2n+1)\,\langle n|n\rangle\Big) \\
&\quad\cdot\Big(\sqrt{(n+1)(n+2)}\,\langle n+2|n+2\rangle + \sqrt{n(n-1)}\,\langle n-2|n-2\rangle + (2n+1)\,\langle n|n\rangle\Big)
\end{aligned}$$

$$\boxed{\langle\psi_n|x^4|\psi_n\rangle = \frac{\hbar^2}{2m^2\omega^2}\Big(\sqrt{n(n-1)} + \sqrt{(n+2)(n+1)} + 2n+1\Big)}$$

□

Comment: In Dirac notation, the above procedure is equivalent to adding an identity operator, in the sense that

$$\sum_m |m\rangle\langle m| = I \tag{4.11}$$

and

$$\langle n|\hat{O}_1\hat{O}_2|n\rangle = \langle n|\hat{O}_1 I\hat{O}_2|n\rangle = \sum_m \langle n|\hat{O}_1|m\rangle\ \langle m|\hat{O}_2|n\rangle = \sum_m O_{1,nm}O_{2,mn} \tag{4.12}$$

3. In class, and in PSet 3, we computed the time dependence of the mean value of $\hat{x}$ in a harmonic oscillator and showed that it had some resemblance with the classical case. Use your preferred computational code language and the form of the energy eigenstate solutions in terms of Hermite polynomials and Gaussian factors to compute the variation of the mean value of the position as a function of time for different coefficients c_n with

$$\Psi(x,t) = \sum_n c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar} \tag{4.13}$$

Additionally, demonstrate numerically that — as expected — it always moves with a classical frequency ω such that $E_n = \hbar\omega(n+1/2)$. Compute also the value of $|\psi(x,t)|^2$ and draw it for different times to show that its shape does not vary over a period of time and is also recovered after half a period but for the opposite values of x, i.e.,

$$|\psi(x,t+T/2)|^2 = |\psi(-x,t)|^2 \tag{4.14}$$

Hint: This is shown analytically in Wagner's notes.

Do this also for a coherent state where $c_{n+1}/c_n = 1/\sqrt{n+1}$. In order to perform this computation, define $\hbar = 1 = m = \omega$ and don't worry about the overall normalization. You may use for guidance the Mathematica code that is posted on Canvas and which does some of this.