

# PHYS 23410 (Quantum Mechanics I) Problem Sets

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# 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**

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

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  $\psi$  with its complex conjugate  $\psi^*$ . 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.

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

□

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  $V \rightarrow \mathbb{C}^3$ , 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.  $\square$

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

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

- 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  $u, v : \mathbb{C}^3 \rightarrow \mathbb{C}$  be functions with smoothness constraints analogous to  $\psi$ . As in the one-dimensional case, we'll start with the product rule and integrate.

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

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

$$\begin{aligned} \int d^3\vec{r} \psi^* \left( -\hbar^2 \vec{\nabla}^2 \psi \right) &= - \int d^3\vec{r} \underbrace{\hbar\psi^*}_u \underbrace{\vec{\nabla}^2(\hbar\psi)}_{\vec{\nabla}^2 v} \\ &= - \underbrace{\int_{\Omega} \vec{\nabla} \cdot [(\hbar\psi^*) \vec{\nabla}(\hbar\psi)]}_0 + \int d^3\vec{r} \vec{\nabla}(\hbar\psi^*) \cdot \vec{\nabla}(\hbar\psi) \\ &= \int d^3\vec{r} |\vec{\nabla}(\hbar\psi)|^2 \end{aligned}$$

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

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

Essentially, this means that the original integral is equal to an integral of an integrand containing  $\psi^*$  (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  $d\Omega$  approaches the “boundary” of  $\mathbb{C}^3$  — is zero, justifying the original substitution.  $\square$

- b) Now consider the expectation value of the Hamiltonian  $\hat{p}^2/2m + V(\vec{r}, t)$  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  $(\hat{p}^2/2m)\psi = (E - V)\psi$ , 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

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

$> 0$

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

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

where  $\psi_m$  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

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

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

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

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

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

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  $\delta_{ij}$  is the **Kronecker delta**. Do it for the mean value of the commutator in a particular state with wave function  $\psi_n$ .

*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

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

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.

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

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<sup>[1]</sup>.  $\square$

<sup>[1]</sup>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

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

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

$$\begin{aligned} V(x) &\rightarrow \infty & \text{for } x \leq 0 \text{ and } x \geq a \\ V(x) &\rightarrow 0 & \text{for } 0 < x < a \end{aligned} \quad (2.2)$$

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

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

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

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (2.4)$$

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

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

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

$$\begin{aligned} 1 &= \langle\psi|\psi\rangle \\ &= \langle c_1\psi_1 + c_3\psi_3 + c_5\psi_5 | c_1\psi_1 + c_3\psi_3 + c_5\psi_5 \rangle \\ &= \langle c_1\psi_1 | c_1\psi_1 \rangle + \langle c_3\psi_3 | c_3\psi_3 \rangle + \langle c_5\psi_5 | c_5\psi_5 \rangle + 2 \underbrace{\langle c_1\psi_1 | c_3\psi_3 \rangle}_0 + 2 \underbrace{\langle c_1\psi_1 | c_5\psi_5 \rangle}_0 + 2 \underbrace{\langle c_3\psi_3 | c_5\psi_5 \rangle}_0 \\ &= \langle c_1\psi_1 | c_1\psi_1 \rangle + \langle c_3\psi_3 | c_3\psi_3 \rangle + \langle c_5\psi_5 | c_5\psi_5 \rangle \\ &= \int_0^a \frac{A^2}{a} \sin^2\left(\frac{\pi x}{a}\right) dx + \int_0^a \frac{3}{5a} \sin^2\left(\frac{3\pi x}{a}\right) dx + \int_0^a \frac{1}{5a} \sin^2\left(\frac{5\pi x}{a}\right) dx \\ &= \frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} \\ &= \frac{5A^2 + 4}{10} \end{aligned}$$

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

□



- 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

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

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

$$P_1 = \frac{3}{5} \quad P_3 = \frac{3}{10} \quad P_5 = \frac{1}{10}$$

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

$$\langle E \rangle = E_1P_1 + E_3P_3 + E_5P_5$$

$$\langle E \rangle = \frac{29\hbar^2\pi^2}{10ma^2}$$

□

- 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

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

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

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

Therefore,

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

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

□

- 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

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

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.

Taking the hint, we may observe that  $\psi(x, t)$  is the sum of wave functions which all have odd  $n$ , meaning that they are each even about the center point  $x = a/2$  of the well. Thus, the entire wave function is even about  $a/2$ . Since the product of an odd and an even function is an odd function, we consequently have that

$$\begin{aligned} \langle \psi(x, t) | \hat{x} | \psi(x, t) \rangle &= \int_0^a x |\psi(x, t)|^2 dx \\ &= \underbrace{\int_0^a \left(x - \frac{a}{2}\right) |\psi(x, t)|^2 dx}_0 + \frac{a}{2} \underbrace{\int_0^a |\psi(x, t)|^2 dx}_1 \\ &= \frac{a}{2} \end{aligned}$$

Just to clarify,  $x - a/2$  is odd with respect to the center of the well and  $|\psi(x, t)|^2$  is even, so their product is odd. The integral of an odd function over all space is always zero. For the right term, the normalization requirement evaluates it to 1.

The above constant clearly has zero derivative with respect to time. It therefore follows by what we said at the beginning that the mean value of the position operator is independent of time.

As to the second part of the question, we have that

$$\langle \psi(x, t) | \hat{p} | \psi(x, t) \rangle = m \frac{d}{dt} (\underbrace{\langle \psi(x, t) | \hat{x} | \psi(x, t) \rangle}_0) = 0$$

Therefore, the mean value of the momentum operator is independent of time. □

- e) Would the result of part (d) be different if we replaced  $\psi_3$  by  $\psi_2$  in Eq. 2.5?

*Answer.* If we replace  $\psi_3$  by  $\psi_2$ , then  $\psi(x, t)$  will have no definite parity (will be neither even nor odd). Thus, the left integral in part (d) will no longer vanish generically; instead, it will be some function of time. This will also affect the momentum result since it follows from the position result. So overall, yes the result will be different. □

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

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

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

$$\psi_1(x) = S_1 \sin(k_1 x) + C_1 \cos(k_1 x) \quad \psi_2(x) = S_2 \sin(k_2 x) + C_2 \cos(k_2 x)$$

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

$$\begin{aligned} \psi_1(0) &= \psi_2(0) \\ C_1 &= C_2 \end{aligned}$$

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

$$\begin{aligned} \psi'_1(0) &= \psi'_2(0) \\ k_1 S_1 &= k_2 S_2 \end{aligned}$$

If we are to have  $\psi(-a/2) = \psi_1(-a/2) = 0$  at the left boundary, then we must have

$$\begin{aligned} S_1 \sin\left(-\frac{k_1 a}{2}\right) + C_1 \cos\left(-\frac{k_1 a}{2}\right) &= 0 \\ -S_1 \sin\left(\frac{k_1 a}{2}\right) + C_1 \cos\left(\frac{k_1 a}{2}\right) &= 0 \end{aligned}$$

If we are to have  $\psi(a/2) = \psi_2(a/2) = 0$  at the right boundary, then we must have

$$S_2 \sin\left(\frac{k_2 a}{2}\right) + C_2 \cos\left(\frac{k_2 a}{2}\right) = 0$$

Now combining all four boundary condition equations above (and favoring  $C_1, S_1$  over  $C_2, S_2$ ), we obtain the following two equations.

$$S_1 \sin\left(\frac{k_1 a}{2}\right) = C_1 \cos\left(\frac{k_1 a}{2}\right) \quad \frac{k_1 S_1}{k_2} \sin\left(\frac{k_2 a}{2}\right) = -C_1 \cos\left(\frac{k_2 a}{2}\right)$$

Now divide the right equation above by the left one.

$$\begin{aligned} \frac{\frac{k_1 S_1}{k_2} \sin\left(\frac{k_2 a}{2}\right)}{S_1 \sin\left(\frac{k_1 a}{2}\right)} &= -\frac{C_1 \cos\left(\frac{k_2 a}{2}\right)}{C_1 \cos\left(\frac{k_1 a}{2}\right)} \\ \frac{k_1}{k_2} &= -\frac{\sin\left(\frac{k_1 a}{2}\right) \cos\left(\frac{k_2 a}{2}\right)}{\cos\left(\frac{k_1 a}{2}\right) \sin\left(\frac{k_2 a}{2}\right)} \\ \boxed{\frac{k_1}{k_2} = -\tan\left(\frac{k_1 a}{2}\right) \cot\left(\frac{k_2 a}{2}\right)} \end{aligned}$$

Since

$$k_1 = \frac{\sqrt{2mE_n}}{\hbar} \qquad k_2 = \frac{\sqrt{2m(E_n - V_0)}}{\hbar}$$

the above equation gives one constraint on the possible energy states. An additional one can be obtained directly from these equations and is

$$k_2^2 - k_1^2 = -\frac{2mV_0}{\hbar^2}$$

Together, these two equations can (theoretically) be solved for the two variables  $k_1, k_2$  and, thus, for the energy states  $E_n$ .  $\square$

- b) Consider now an energy  $E_n < V_0$ . What is the form of the solution at positive values of  $x$ ?

*Hint:* The solutions at  $x > 0$  are no longer given in terms of sine and cosine functions. They can now be written in terms of exponential functions. You can obtain the new solutions by using the same solutions as for  $E_n > V_0$ , and the known relations between trigonometric and hyperbolic sine and cosine functions, namely  $\sin(ix) = i \sinh(x)$  and  $\cos(ix) = \cosh(x)$ .

In classical mechanics, a particle cannot enter a region where the potential energy is larger than the energy of the particle, since it would imply that the kinetic energy is negative. Is this still true in quantum mechanics? In other words, does the probability of finding the particle at positive values of  $x$  vanish?

*Answer.* We first define the Schrödinger equation at positive values of  $x$  in this case.

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V_0\psi_2 &= E_n\psi_2 \\ \frac{d^2\psi_2}{dx^2} &= \underbrace{\frac{2m(V_0 - E_n)}{\hbar^2}}_{\kappa_2^2} \psi_2 \end{aligned}$$

Taking the hint, the general solution to this equation is

$$\begin{aligned} \psi_2(x) &= Ae^{\kappa_2 x} + Be^{-\kappa_2 x} \\ &= \frac{\tilde{S}_2 + \tilde{C}_2}{2} e^{\kappa_2 x} + \frac{\tilde{C}_2 - \tilde{S}_2}{2} e^{-\kappa_2 x} \\ &= \tilde{S}_2 \cdot \frac{e^{\kappa_2 x} - e^{-\kappa_2 x}}{2} + \tilde{C}_2 \cdot \frac{e^{\kappa_2 x} + e^{-\kappa_2 x}}{2} \\ &= \tilde{S}_2 \sinh(\kappa_2 x) + \tilde{C}_2 \cosh(\kappa_2 x) \\ &= -i\tilde{S}_2 \sin(i\kappa_2 x) + \tilde{C}_2 \cos(i\kappa_2 x) \end{aligned}$$

Now observe that

$$i\kappa_2 = \frac{\sqrt{2m(E_n - V_0)}}{\hbar} = k_2$$

Additionally, define

$$S_2 := -i\tilde{S}_2 \qquad C_2 := \tilde{C}_2$$

Thus,

$$\psi_2(x) = S_2 \sin(k_2 x) + C_2 \cos(k_2 x)$$

Additionally, we still have that

$$\psi_1(x) = S_1 \sin(k_1 x) + C_1 \cos(k_1 x)$$

so the boundary conditions at  $x = 0$  imply by transitivity that

$$C_1 = C_2 = \tilde{C}_2 \quad k_1 S_1 = k_2 S_2 = (i\kappa_2)(-i\tilde{S}_2) = \kappa_2 \tilde{S}_2$$

Since  $\psi_2$  will vanish if and only if  $\tilde{S}_2 = \tilde{C}_2 = 0$ , the above two equations imply that in this case,  $S_1 = C_1 = 0$ , too. Therefore, in general, it is not still true in quantum mechanics that a particle cannot enter a region where the potential energy is larger than the energy of the particle. In other words, the probability of finding the particle at positive values of  $x$  does not vanish.  $\square$

- c) What happens when  $V_0 \rightarrow \infty$ ? In principle, one obtains in this limit an infinite square well of length  $a/2$ . Hence, the energy eigenstates should change such that

$$\sin\left(\frac{k_n a}{2}\right) = 0 \quad (2.7)$$

with

$$\frac{\hbar^2 k_n^2}{2m} = E_n \quad (2.8)$$

Is this true? What happens to the wave function at positive values of  $x$ ?

*Answer.* Here, it will be convenient to write

$$\psi_2(x) = Ae^{\kappa_2 x} + Be^{-\kappa_2 x}$$

Now since  $\kappa_2 \propto V_0^{1/2}$ , as  $V_0 \rightarrow \infty$ ,  $\kappa_2 \rightarrow \infty$ . Thus, to keep  $\psi_2$  from blowing up at positive  $x$ , we must set  $A = 0$ . Additionally, we will have  $e^{-\kappa_2 x} \rightarrow 0$  so that at  $V_0 = \infty$ ,

$$\psi_2(x) = 0$$

Additionally, the boundary conditions at zero (and the fact that  $A = 0$ ) imply that

$$\begin{aligned} \psi_1(0) &= \psi_2(0) & \psi_1'(0) &= \psi_2'(0) \\ C_1 &= B & k_1 S_1 &= -\kappa_2 B \end{aligned}$$

Therefore, our last boundary condition gives us that

$$\begin{aligned} 0 &= \psi_1\left(-\frac{a}{2}\right) \\ &= S_1 \sin\left(-\frac{k_1 a}{2}\right) + C_1 \cos\left(-\frac{k_1 a}{2}\right) \\ &= -S_1 \sin\left(\frac{k_1 a}{2}\right) + C_1 \cos\left(\frac{k_1 a}{2}\right) \\ &= \frac{\kappa_2 B}{k_1} \sin\left(\frac{k_1 a}{2}\right) + B \cos\left(\frac{k_1 a}{2}\right) \\ &= \sin\left(\frac{k_1 a}{2}\right) + \frac{k_1}{\kappa_2} \cos\left(\frac{k_1 a}{2}\right) \\ &= \sin\left(\frac{k_1 a}{2}\right) + \frac{k_1}{\infty} \cos\left(\frac{k_1 a}{2}\right) \\ &= \sin\left(\frac{k_1 a}{2}\right) \\ \frac{k_1 a}{2} &= \pi n \\ \frac{\sqrt{2mE_n}}{\hbar} &= \frac{2\pi n}{a} \\ E_n &= \frac{\hbar^2 \pi^2 n^2}{2m(a/2)^2} \end{aligned}$$

as desired. So yes, it is true.  $\square$

3. Although planar waves are not well normalized, one can use them to demonstrate the tunneling phenomenon. Note that a well-normalized solution would be a wave packet of these planar waves, namely

$$\psi(x, 0) = \frac{1}{\sqrt{2\pi}} \int dk \Phi(k) e^{ikx} \quad (2.9)$$

Consider a stationary solution of a free particle with finite energy  $E$  and forget for the time being the question of normalization. The momentum of the particle will be given by  $|\hbar k| = \sqrt{E/2m}$  and

$$\psi(x, t) = Ae^{i(kx - \omega t)} + Be^{i(-kx - \omega t)} \quad (2.10)$$

with  $\hbar\omega = E$ .

Observe that there are two solutions, one with positive (incoming wave) and the other with negative (reflected wave) values of the momentum in the  $x$ -direction. In the previous problems, they combined to give sine and cosine functions due to the boundary conditions. Now, imagine that we consider that this particle goes through a potential

$$\begin{aligned} V(x) &= 0 & \text{for } |x| > a/2 \\ V(x) &= V_0 & \text{for } |x| \leq a/2 \end{aligned} \quad (2.11)$$

Since we want to consider the transmission of the particle at the right of the potential barrier, consider the case in which at the right of this finite potential barrier, the wave function is described by a particle moving freely in the positive direction of  $x$  via

$$\psi(x, t) = Ce^{i(kx - \omega t)} \quad (2.12)$$

for  $x > a/2$  while for  $x < -a/2$ , we have the function given in Eq. 2.10. The ratio  $|B/A|^2$  may be considered as the reflection probability, while  $|C/A|^2$  is the transmission probability.

The solutions for  $-a/2 \leq x \leq a/2$ , instead, are given by

$$\psi(x, t) = Fe^{i(k_2x - \omega t)} + Ge^{i(-k_2x - \omega t)} \quad (2.13)$$

with  $k_2 = \sqrt{2m(E - V_0)}/\hbar$ . Observe that  $\omega$  is unchanged.

Using continuity of the wave function and its derivatives at  $x = \pm a/2$ , calculate the reflection and transmission probabilities. Consider both the case of  $E > V_0$  and  $E < V_0$ , and try to interpret the results. What happens when  $V_0 \rightarrow \infty$ ?

*Answer.* The total spatial wave function is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -\frac{a}{2} \\ Fe^{ik_2x} + Ge^{-ik_2x} & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ Ce^{ikx} & \frac{a}{2} < x \end{cases}$$

For now, we will remain agnostic about whether  $E > V_0$  or  $E < V_0$ , since in the latter case,  $k_2$  will just become imaginary so that the solutions in the middle region are real exponentials.

As recommended, we begin with the equations given by the continuity of  $\psi$  and its derivatives at the  $\pm a/2$  boundaries. For continuity, we have

$$\begin{aligned} \psi_1(-a/2) &= \psi_2(-a/2) & \psi_2(a/2) &= \psi_3(a/2) \\ Ae^{-ika/2} + Be^{ika/2} &= Fe^{-ik_2a/2} + Ge^{ik_2a/2} & Fe^{ik_2a/2} + Ge^{-ik_2a/2} &= Ce^{ika/2} \end{aligned}$$

For continuity of the first derivative, we have

$$\begin{aligned} \psi'_1(-a/2) &= \psi'_2(-a/2) & \psi'_2(a/2) &= \psi'_3(a/2) \\ k(Ae^{-ika/2} - Be^{ika/2}) &= k_2(Fe^{-ik_2a/2} - Ge^{ik_2a/2}) & k_2(Fe^{ik_2a/2} - Ge^{-ik_2a/2}) &= kCe^{ika/2} \end{aligned}$$

We now algebraically manipulate the above four equations until we arrive at the final answer.

To begin, adding the left two boundary conditions gives

$$A \left(1 + \frac{k}{k_2}\right) e^{-ika/2} + B \left(1 - \frac{k}{k_2}\right) e^{ika/2} = 2F e^{-ik_2a/2}$$

while subtracting them gives

$$A \left(1 - \frac{k}{k_2}\right) e^{-ika/2} + B \left(1 + \frac{k}{k_2}\right) e^{ika/2} = 2G e^{ik_2a/2}$$

Additionally, adding the right two boundary conditions gives

$$C \left(1 + \frac{k}{k_2}\right) e^{ika/2} = 2F e^{ik_2a/2}$$

while subtracting them gives

$$C \left(1 - \frac{k}{k_2}\right) e^{ika/2} = 2G e^{-ik_2a/2}$$

It follows by consecutive applications of the transitivity property that

$$A \left(1 + \frac{k}{k_2}\right) e^{-ika/2} + B \left(1 - \frac{k}{k_2}\right) e^{ika/2} = C \left(1 + \frac{k}{k_2}\right) e^{ika/2} e^{-ik_2a}$$

and

$$A \left(1 - \frac{k}{k_2}\right) e^{-ika/2} + B \left(1 + \frac{k}{k_2}\right) e^{ika/2} = C \left(1 - \frac{k}{k_2}\right) e^{ika/2} e^{ik_2a}$$

Now divide through both of the above equations by the first term to yield

$$\begin{aligned} 1 + \underbrace{\left(\frac{B}{A}\right)}_r \underbrace{\left(\frac{1 - k/k_2}{1 + k/k_2}\right)}_\alpha e^{ika} &= \underbrace{\left(\frac{C}{A}\right)}_t e^{i(k-k_2)a} \\ 1 + \underbrace{\left(\frac{B}{A}\right)}_r \underbrace{\left(\frac{1 + k/k_2}{1 - k/k_2}\right)}_{\alpha^{-1}} e^{ika} &= \underbrace{\left(\frac{C}{A}\right)}_t e^{i(k+k_2)a} \end{aligned}$$

Making the suggested substitutions for convenience, we obtain

$$1 + r\alpha e^{ika} = t e^{i(k-k_2)a} \qquad 1 + r\alpha^{-1} e^{ika} = t e^{i(k+k_2)a}$$

This system of two equations is linear in  $r$  and  $t$  and hence can easily be solved for these variables by formula. In particular, it is a fact of algebra that the solution to  $1 + xA = yB$  and  $1 + xC = yD$  is  $x = (D - B)/(BC - AD)$  and  $y = (C - A)/(BC - AD)$ .<sup>[2]</sup> Thus,

$$\begin{aligned} r &= \frac{e^{i(k+k_2)a} - e^{i(k-k_2)a}}{[e^{i(k-k_2)a}][\alpha^{-1}e^{ika}] - [\alpha e^{ika}][e^{i(k+k_2)a}]} & t &= \frac{\alpha^{-1}e^{ika} - \alpha e^{ika}}{[e^{i(k-k_2)a}][\alpha^{-1}e^{ika}] - [\alpha e^{ika}][e^{i(k+k_2)a}]} \\ &= \frac{e^{ika}e^{ik_2a} - e^{ika}e^{-ik_2a}}{\alpha^{-1}e^{ika}e^{-ik_2a}e^{ika} - \alpha e^{ika}e^{ika}e^{ik_2a}} & &= \frac{\alpha^{-1}e^{ika} - \alpha e^{ika}}{\alpha^{-1}e^{ika}e^{-ik_2a}e^{ika} - \alpha e^{ika}e^{ika}e^{ik_2a}} \\ &= \frac{e^{ik_2a} - e^{-ik_2a}}{(\alpha^{-1}e^{-ik_2a} - \alpha e^{ik_2a})e^{ika}} & &= \frac{\alpha^{-1} - \alpha}{(\alpha^{-1}e^{-ik_2a} - \alpha e^{ik_2a})e^{ika}} \\ &= \frac{2i \sin(k_2a)}{(\alpha^{-1}e^{-ik_2a} - \alpha e^{ik_2a})e^{ika}} & &= \frac{1 - \alpha^2}{(e^{-ik_2a} - \alpha^2 e^{ik_2a})e^{ika}} \end{aligned}$$

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<sup>2</sup>This fact can be readily verified by direct substitution. It can be derived via elimination of the original equations.

Thus, we may finally obtain the reflection and transmission coefficients<sup>[3]</sup> via

$$\begin{aligned}
 |r|^2 &= r^* \cdot r \\
 &= \frac{-2i \sin(k_2 a)}{(\alpha^{-1} e^{ik_2 a} - \alpha e^{-ik_2 a}) e^{-ika}} \cdot \frac{2i \sin(k_2 a)}{(\alpha^{-1} e^{-ik_2 a} - \alpha e^{ik_2 a}) e^{ika}} \\
 &= \frac{4 \sin^2(k_2 a)}{(\alpha^{-1} e^{ik_2 a} - \alpha e^{-ik_2 a}) \cdot (\alpha^{-1} e^{-ik_2 a} - \alpha e^{ik_2 a})} \\
 &= \frac{4 \sin^2(k_2 a)}{\alpha^{-2} - e^{2ik_2 a} - e^{-2ik_2 a} + \alpha^2} \\
 &= \frac{4\alpha^2 \sin^2(k_2 a)}{1 + \alpha^4 - \alpha^2(e^{2ik_2 a} + e^{-2ik_2 a})}
 \end{aligned}$$

$$|B/A|^2 = \frac{4\alpha^2 \sin^2(k_2 a)}{1 + \alpha^4 - 2\alpha^2 \cos(2k_2 a)}$$

and

$$\begin{aligned}
 |t|^2 &= t^* \cdot t \\
 &= \frac{1 - \alpha^2}{(e^{ik_2 a} - \alpha^2 e^{-ik_2 a}) e^{-ika}} \cdot \frac{1 - \alpha^2}{(e^{-ik_2 a} - \alpha^2 e^{ik_2 a}) e^{ika}} \\
 &= \frac{(1 - \alpha^2)^2}{(e^{ik_2 a} - \alpha^2 e^{-ik_2 a}) \cdot (e^{-ik_2 a} - \alpha^2 e^{ik_2 a})} \\
 &= \frac{(1 - \alpha^2)^2}{1 - \alpha^2 e^{2ik_2 a} - \alpha^2 e^{-2ik_2 a} + \alpha^4} \\
 &= \frac{(1 - \alpha^2)^2}{1 + \alpha^4 - \alpha^2(e^{2ik_2 a} + e^{-2ik_2 a})}
 \end{aligned}$$

$$|C/A|^2 = \frac{(1 - \alpha^2)^2}{1 + \alpha^4 - 2\alpha^2 \cos(2k_2 a)}$$

At this point, we will cease our agnosticism regarding the parity of  $E - V_0$ . The answers above correspond to the case that  $E > V_0$ . In the case that  $E < V_0$ , we fortunately need only make minor adjustments to the above. In particular, we define the real value  $\kappa := \sqrt{2m(V_0 - E)}/\hbar$  so that we may write  $k_2 = i\kappa$  and use the imaginary hyperbolic sine and cosine functions from Q2b to yield

$$\begin{aligned}
 |B/A|^2 &= \frac{4\alpha^2 [\sin(i\kappa a)]^2}{1 + \alpha^4 - 2\alpha^2 \cos(i2\kappa a)} \\
 &= \frac{4\alpha^2 [i \sinh(\kappa a)]^2}{1 + \alpha^4 - 2\alpha^2 \cosh(2\kappa a)}
 \end{aligned}$$

$$|C/A|^2 = \frac{(1 - \alpha^2)^2}{1 + \alpha^4 - 2\alpha^2 \cos(i2\kappa a)}$$

$$|C/A|^2 = \frac{(1 - \alpha^2)^2}{1 + \alpha^4 - 2\alpha^2 \cosh(2\kappa a)}$$

$$|B/A|^2 = \frac{-4\alpha^2 \sinh^2(\kappa a)}{1 + \alpha^4 - 2\alpha^2 \cosh(2\kappa a)}$$

Lastly, we consider the case where  $V_0 \rightarrow \infty$ . In this case,  $V_0$  will eventually exceed any value of  $E$ , so we will work with the second pair of equations defining the reflection and transmission coefficients. To begin, observe that by definition,  $\kappa \propto V_0^{1/2}$ . Thus, as  $V_0 \rightarrow \infty$ ,  $\kappa \rightarrow \infty$  and, in particular,

$$\alpha = \frac{1 - k/i\kappa}{1 + k/i\kappa} = \frac{i - k/\kappa}{i + k/\kappa} \rightarrow \frac{i - k/\infty}{i + k/\infty} = \frac{i}{i} = i \cdot (-i) = 1$$

Thus, by the form of the numerator of  $|C/A|^2$ ,  $|C/A|^2 \rightarrow 0$ . But this must imply that  $|B/A|^2 \rightarrow 1$ . That is, there is no tunneling and the particle is completely reflected.  $\square$

<sup>3</sup>Note that a good sanity check for the following answers is that they sum to 1.



### 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

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

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

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

with  $g = 9.8 \text{ m/s}^2$  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  $x_{\text{eq}}$  will correspond to a minimum of  $V$ . Thus, we may solve

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

for  $x_{\text{eq}}$ . Doing this, we obtain

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

$$\boxed{x_{\text{eq}} = -\frac{g}{\omega^2}}$$

Let

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

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

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

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 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  $\psi_n^{\text{HO}}$  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  $\psi_n$  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  $E_n, \psi_n$ , we must solve the following ODE.

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

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.

$$\begin{aligned} & -\frac{\hbar^2}{2m} \frac{d}{dx} \left[ \frac{d}{dx} \psi_n(u) \right] + \frac{m\omega^2 u^2}{2} \psi_n(u) = E_n \psi_n(u) \\ & -\frac{\hbar^2}{2m} \frac{d}{dx} \left[ \frac{d}{du} \psi_n(u) \cdot \underbrace{\frac{du}{dx}}_1 \right] + \frac{m\omega^2 u^2}{2} \psi_n(u) = E_n \psi_n(u) \\ & -\frac{\hbar^2}{2m} \frac{d}{du} \left[ \frac{d}{du} \psi_n(u) \right] \cdot \underbrace{\frac{du}{dx}}_1 + \frac{m\omega^2 u^2}{2} \psi_n(u) = E_n \psi_n(u) \\ & -\frac{\hbar^2}{2m} \frac{d^2}{du^2} \psi_n(u) + \frac{m\omega^2 u^2}{2} \psi_n(u) = E_n \psi_n(u) \end{aligned}$$

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

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

It follows by returning the substitution that

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

□

- 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  $x_{\text{eq}}$  is the equilibrium point.

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

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

In the ground state of the system, we have (taking the hint) that

$$\begin{aligned} \langle \psi_0 | \hat{x}^2 | \psi_0 \rangle &= \int \psi_0^*(x) x^2 \psi_0(x) dx \\ &= \int [\psi_0^{\text{HO}}]^*(u) (x_{\text{eq}} + u)^2 \psi_0^{\text{HO}}(u) du \\ &= x_{\text{eq}}^2 \int [\psi_0^{\text{HO}}]^*(u) \psi_0^{\text{HO}}(u) du + 2x_{\text{eq}} \int [\psi_0^{\text{HO}}]^*(u) u \psi_0^{\text{HO}}(u) du \\ &\quad + \int [\psi_0^{\text{HO}}]^*(u) u^2 \psi_0^{\text{HO}}(u) du \end{aligned}$$

The leftmost integral above evaluates to 1. The middle integral above evaluates to zero because its integrand is an odd function (the product of an odd and even function). The right integral expands to

$$\int_{-\infty}^{\infty} u^2 \left( \frac{m\omega}{\hbar\pi} \right)^{1/2} e^{-m\omega u^2/\hbar} du = \frac{\hbar}{2m\omega}$$

upon plugging in the harmonic oscillator's ground state wave function, and may be evaluated using computational software. Thus, altogether,

$$\langle \psi_0 | \hat{x}^2 | \psi_0 \rangle = x_{\text{eq}}^2 + \frac{\hbar}{2m\omega}$$

Similar explicit computations for the mean value of  $p^2$  yield

$$\langle \psi_0 | \hat{p}^2 | \psi_0 \rangle = \frac{\hbar m\omega}{2}$$

□

- 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?

*Answer.* We have that

$$\sigma_x^2 = \langle \psi_0 | \hat{x}^2 | \psi_0 \rangle - (\langle \psi_0 | \hat{x} | \psi_0 \rangle)^2 = x_{\text{eq}}^2 + \frac{\hbar}{2m\omega} - x_{\text{eq}}^2 = \frac{\hbar}{2m\omega}$$

and

$$\sigma_p^2 = \langle \psi_0 | \hat{p}^2 | \psi_0 \rangle - (\langle \psi_0 | \hat{p} | \psi_0 \rangle)^2 = \frac{\hbar m\omega}{2}$$

Therefore, the value of  $\sigma_x \sigma_p$  in the ground state of this system is

$$\begin{aligned} \sigma_x^2 \cdot \sigma_p^2 &= \frac{\hbar}{2m\omega} \cdot \frac{\hbar m\omega}{2} \\ &= \frac{\hbar^2}{4} \\ \sigma_x \sigma_p &= \frac{\hbar}{2} \end{aligned}$$

This does not differ from the value we obtained in the absence of gravity in class on 1/22. □

## 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

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

where  $x_{\text{eq}}$  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.

*Answer.* The motion will be identical for  $x \geq x_{\text{eq}}$ , but instead of continuing past  $x_{\text{eq}}$ , the particle will elastically reflect back. Mathematically, if motion in Q1a was described by

$$x(t) = A \sin(\omega t) + B \cos(\omega t) + x_{\text{eq}}$$

then motion now is described by

$$x(t) = |A \sin(\omega t) + B \cos(\omega t)| + x_{\text{eq}}$$

□

- 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?

*Answer.* At and below  $x = x_{\text{eq}}$ , the potential goes to infinity, so just like in the infinite square well, the particle no longer has a probability of existing there so the wave function must go to zero. □

- 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  $\psi_n$  to this problem. *Hint:* Observe that the boundary condition at  $x = x_{\text{eq}}$  eliminates some solutions.

*Answer.* The Schrödinger equation for positive values of the displacement with respect to the equilibrium point does not change from the one we had without the floor because the potential in that region has not changed.

Since the Schrödinger equation does not change, we can solve it as in Q1b. However, taking the hint, only the odd solutions will be allowed by the boundary condition. Additionally, allowable space has halved from  $(-\infty, \infty)$  to  $[x_{\text{eq}}, \infty)$ , so we must renormalize the odd eigenstates. Fortunately, this is fairly straightforward since  $|\psi_n|^2$  is even, so

$$\begin{aligned} 1 &= \int_{x_{\text{eq}}}^{\infty} |\psi_n(x - x_{\text{eq}})|^2 dx \\ &= \frac{1}{2} \int_{-\infty}^{\infty} |\psi_n(x - x_{\text{eq}})|^2 dx \\ &= \frac{1}{2} \int_{-\infty}^{\infty} |A \psi_n^{\text{HO}}(x - x_{\text{eq}})|^2 dx \\ 2 &= A^2 \\ A &= \sqrt{2} \end{aligned}$$

Thus, the energy eigenvalues and corresponding functions are

$$\psi_n(x) = \sqrt{2} \psi_n^{\text{HO}}(x - x_{\text{eq}}) \quad E_n = E_n^{\text{HO}} + C \quad n = 1, 3, 5, \dots$$

□

- 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?

*Answer.* The minimal energy is now that which corresponds to the new smallest eigenstate, i.e.,

$$E_1 = \frac{3\hbar\omega}{2} + C$$

This is not the same as the system without the floor, which had minimal energy  $\hbar\omega/2 + C$ . The corresponding eigenfunction is  $\psi_1(x)$ . □

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

*Answer.* Per part (d), the minimum energy solution is the wave function

$$\begin{aligned}
 \psi_1(x) &= \sqrt{2}\psi_1^{\text{HO}}(x - x_{\text{eq}}) \\
 &= \sqrt{2} \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{H_1(\xi)}{\sqrt{2^1 1!}} e^{-\xi^2/2} \\
 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \left[(-1)^1 e^{\xi^2} \cdot \frac{d}{d\xi} (e^{-\xi^2})\right] e^{-\xi^2/2} \\
 &= \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \left[-e^{\xi^2} \cdot -2\xi e^{-\xi^2}\right] e^{-\xi^2/2} \\
 &= 2 \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \xi e^{-\xi^2/2} \\
 &= 2 \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} u \left(\frac{m\omega}{\hbar}\right)^{1/2} e^{-m\omega u^2/2\hbar} \\
 &= \frac{2}{\pi^{1/4}} \left(\frac{m\omega}{\hbar}\right)^{3/4} (x - x_{\text{eq}}) e^{-m\omega(x-x_{\text{eq}})^2/2\hbar}
 \end{aligned}$$

From here, we can use computational software to learn that

$$\begin{aligned}
 \langle \psi_1 | \hat{x} | \psi_1 \rangle &= \int_{x_{\text{eq}}}^{\infty} x \psi_1^2(x) dx = \int_0^{\infty} (u + x_{\text{eq}}) \psi_1^2(u + x_{\text{eq}}) du = 2\sqrt{\frac{\hbar}{m\omega\pi}} + x_{\text{eq}} \\
 \langle \psi_1 | \hat{x}^2 | \psi_1 \rangle &= x_{\text{eq}}^2 + \frac{3\hbar}{2m\omega} + 4x_{\text{eq}}\sqrt{\frac{\hbar}{m\omega\pi}} \\
 \langle \psi_1 | \hat{p} | \psi_1 \rangle &= 0 \\
 \langle \psi_1 | \hat{p}^2 | \psi_1 \rangle &= \frac{3\hbar m\omega}{2}
 \end{aligned}$$

Thus,

$$\sigma_x^2 = \left( x_{\text{eq}}^2 + \frac{3\hbar}{2m\omega} + 4x_{\text{eq}}\sqrt{\frac{\hbar}{m\omega\pi}} \right) - \left( 2\sqrt{\frac{\hbar}{m\omega\pi}} + x_{\text{eq}} \right)^2 = \frac{3\hbar}{2m\omega} - \frac{4\hbar}{m\omega\pi}$$

and

$$\sigma_p^2 = \frac{3\hbar m\omega}{2}$$

so

$$\sigma_x\sigma_p = \sqrt{\left(\frac{3\hbar}{2m\omega} - \frac{4\hbar}{m\omega\pi}\right) \left(\frac{3\hbar m\omega}{2}\right)} = \hbar\sqrt{\frac{9}{4} - \frac{6}{\pi}} \approx 0.58\hbar$$

Since  $0.58\hbar \neq \hbar/2$  (the answer to Q1d), no,  $\sigma_x\sigma_p$  is not 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  $\psi_n$ .

*Answer.* We have that

$$\begin{aligned}\langle \psi_n | \hat{x} | \psi_n \rangle &= \sqrt{\frac{\hbar}{2m\omega}} [\langle \psi_n | a_+ | \psi_n \rangle + \langle \psi_n | a_- | \psi_n \rangle] \\ &= \sqrt{\frac{\hbar}{2m\omega}} [\sqrt{n+1} \underbrace{\langle \psi_n | \psi_{n+1} \rangle}_0 + \sqrt{n} \underbrace{\langle \psi_n | \psi_{n-1} \rangle}_0]\end{aligned}$$

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

and

$$\begin{aligned}\langle \psi_n | \hat{p} | \psi_n \rangle &= i\sqrt{\frac{\hbar m\omega}{2}} [\langle \psi_n | a_+ | \psi_n \rangle - \langle \psi_n | a_- | \psi_n \rangle] \\ &= i\sqrt{\frac{\hbar m\omega}{2}} [\sqrt{n+1} \underbrace{\langle \psi_n | \psi_{n+1} \rangle}_0 - \sqrt{n} \underbrace{\langle \psi_n | \psi_{n-1} \rangle}_0]\end{aligned}$$

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

□

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

*Answer.* As derived in class,<sup>[4]</sup> we have that

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

Therefore,

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

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

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

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

□

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

*Answer.* Since<sup>[5]</sup>

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

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.

<sup>4</sup>For future reference, they would have liked me to show this derivation and I did lose points for just stating this result.

<sup>5</sup>There is an entirely different derivation of these facts in the solutions key; one that works directly from the formal commutator definition of the uncertainty principle. Pretty cool!

*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.  $\square$

- 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  $\psi_n$ .

*Hint:* For instance, the mean value of the operators  $x^q$  and  $p^q$  can be obtained by computing

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

and

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

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

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

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

*Answer.* See Lecture 4.2.  $\square$

## 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

$$\frac{d}{dt}(\langle \psi | \hat{p}^n | \psi \rangle) = 0 \quad (4.1)$$

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

*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  $d\langle \psi | \hat{x} | \psi \rangle / dt$ , and show that

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

*Answer.* We have from Lecture 1.2 that

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

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,

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

It follows by integrating that

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

as desired. □



c) Show also that

$$\frac{d}{dt}(\langle \psi | \hat{x}^2 | \psi \rangle) = \frac{2}{m} \langle \psi | \hat{p} \hat{x} | \psi \rangle + \frac{i\hbar}{m} \quad (4.3)$$

*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

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

as desired. □

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

$$\frac{d^2}{dt^2}(\langle \psi | \hat{x}^2 | \psi \rangle) \quad \frac{d^2}{dt^2}[(\langle \psi | \hat{x} | \psi \rangle)^2] \quad (4.4)$$

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

*Answer.* By part (c), we have that

$$\begin{aligned} \frac{d^2}{dt^2}(\langle \psi | \hat{x}^2 | \psi \rangle) &= \frac{2}{m} \frac{d}{dt}(\langle \psi | \hat{p}\hat{x} | \psi \rangle) \\ &= \frac{2i}{m\hbar} \langle \psi | [\hat{H}, \hat{p}\hat{x}] | \psi \rangle \\ &= \frac{i}{m^2\hbar} (\langle \psi | \hat{p}^2 \underbrace{[\hat{p}, \hat{x}]}_{-i\hbar} | \psi \rangle + \langle \psi | \hat{p} \underbrace{[\hat{p}, \hat{p}]}_0 \hat{x} | \psi \rangle + \langle \psi | \hat{p} \underbrace{[\hat{p}, \hat{x}]}_{-i\hbar} \hat{p} | \psi \rangle + \langle \psi | \underbrace{[\hat{p}, \hat{p}]}_0 \hat{x}\hat{p} | \psi \rangle) \end{aligned}$$

$$\frac{d^2}{dt^2}(\langle \psi | \hat{x}^2 | \psi \rangle) = \frac{2}{m^2} \langle \psi | \hat{p}^2 | \psi \rangle$$

By part (b), we have that

$$\begin{aligned}
 \frac{d^2}{dt^2} [(\langle \psi | \hat{x} | \psi \rangle)^2] &= \frac{d}{dt} [2 \langle \psi | \hat{x} | \psi \rangle \cdot \frac{d}{dt} (\langle \psi | \hat{x} | \psi \rangle)] \\
 &= 2 \frac{d}{dt} (\langle \psi | \hat{x} | \psi \rangle) \cdot \frac{d}{dt} (\langle \psi | \hat{x} | \psi \rangle) + 2 \langle \psi | \hat{x} | \psi \rangle \cdot \frac{d^2}{dt^2} (\langle \psi | \hat{x} | \psi \rangle) \\
 &= \frac{2p_0^2}{m^2} + 2x_0 \cdot \underbrace{\frac{d}{dt} \left( \frac{p_0}{m} \right)}_0
 \end{aligned}$$

$$\frac{d^2}{dt^2} [(\langle \psi | \hat{x} | \psi \rangle)^2] = \frac{2}{m^2} (\langle \psi | \hat{p} | \psi \rangle)^2$$

□

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

$$\frac{d^2}{dt^2} (\sigma_x^2) = \frac{2\sigma_p^2}{m^2} \quad (4.5)$$

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

$$\sigma_x \approx \frac{\sigma_p t}{m} \quad (4.6)$$

where  $\sigma_p$  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

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

Since  $\sigma_p$  is constant with respect to time — as we may extrapolate from part (a) — the solution to this ODE may be found via integration to be

$$\begin{aligned}
 \frac{d^2}{dt^2} (\sigma_x^2) &= \frac{2\sigma_p^2}{m^2} \\
 \frac{d}{dt} (\sigma_x^2) &= \frac{2\sigma_p^2}{m^2} t + c \\
 \sigma_x^2 &= \frac{\sigma_p^2}{m^2} t^2 + ct + d
 \end{aligned}$$

where  $c, d$  are constants of integration. Moreover, when we make  $t$  sufficiently large, the  $ct + d$  terms are negligible and

$$\begin{aligned}
 \sigma_x^2 &\approx \frac{\sigma_p^2}{m^2} t^2 \\
 \sigma_x &\approx \frac{\sigma_p}{m} t
 \end{aligned}$$

as desired. Additionally, 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.  $\square$

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

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

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

$$\delta(x_1 - x_2) = \sum_m \psi_m(x_1) \psi_m^*(x_2) \quad (4.8)$$

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

$$\int \delta(x_1 - x_2) \psi(x_2) dx_2 = \int \sum_m \psi_m(x_1) \psi_m^*(x_2) \psi(x_2) dx_2$$

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

$$\int \delta(x_1 - x_2) \psi(x_2) dx_2 = \psi(x_1)$$

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

$$\begin{aligned} \int \sum_m \psi_m(x_1) \psi_m^*(x_2) \psi(x_2) dx_2 &= \int \sum_m \psi_m(x_1) \psi_m^*(x_2) \left( \sum_{n=0}^{\infty} c_n \psi_n(x_2) \right) dx_2 \\ &= \sum_m \sum_{n=0}^{\infty} c_n \psi_m(x_1) \int \psi_m^*(x_2) \psi_n(x_2) dx_2 \\ &= \sum_{n=0}^{\infty} c_n \psi_n(x_1) \\ &= \psi(x_1) \end{aligned}$$

Therefore, by transitivity, we have the desired equality.  $\square$

- 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  $\psi_n$ , one needs to compute

$$\langle \psi_n | h(x) | \psi_n \rangle = \int \psi_n^*(x) f(x) g(x) \psi_n(x) dx = \iint \psi_n^*(x_1) f(x_1) \delta(x_1 - x_2) g(x_2) \psi_n(x_2) dx_1 dx_2 \quad (4.9)$$

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

$$\begin{aligned} \text{RHS} &= \iint \psi_n^*(x_1) f(x_1) \delta(x_1 - x_2) g(x_2) \psi_n(x_2) dx_1 dx_2 \\ &= \int \left[ \int \psi_n^*(x_1) f(x_1) \delta(x_1 - x_2) dx_1 \right] g(x_2) \psi_n(x_2) dx_2 \\ &= \int [\psi_n^*(x_2) f(x_2)] g(x_2) \psi_n(x_2) dx_2 \\ &= \int \psi_n^*(x) f(x) g(x) \psi_n(x) dx \\ &= \int \psi_n^*(x) h(x) \psi_n(x) dx \\ &= \langle \psi_n | h(x) | \psi_n \rangle \end{aligned}$$

□

- 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

$$f_{mn} = \int \psi_m^*(x) f(x) \psi_n(x) dx \quad g_{mn} = \int \psi_m^*(x) g(x) \psi_n(x) dx \quad (4.10)$$

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

$$\begin{aligned} \langle \psi_n | h(x) | \psi_n \rangle &= \iint \psi_n^*(x_1) f(x_1) \delta(x_1 - x_2) g(x_2) \psi_n(x_2) dx_1 dx_2 \\ &= \iint \psi_n^*(x_1) f(x_1) \left[ \sum_m \psi_m(x_1) \psi_m^*(x_2) \right] g(x_2) \psi_n(x_2) dx_1 dx_2 \\ &= \sum_m \iint \psi_n^*(x_1) f(x_1) \psi_m(x_1) \psi_m^*(x_2) g(x_2) \psi_n(x_2) dx_1 dx_2 \\ &= \sum_m \int \left[ \int \psi_n^*(x_1) f(x_1) \psi_m(x_1) dx_1 \right] \psi_m^*(x_2) g(x_2) \psi_n(x_2) dx_2 \\ &= \sum_m \int f_{nm} \psi_m^*(x_2) g(x_2) \psi_n(x_2) dx_2 \\ &= \sum_m f_{nm} \int \psi_m^*(x_2) g(x_2) \psi_n(x_2) dx_2 \end{aligned}$$

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

□

- 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 (c), we have that

$$\langle \psi_n | x^4 | \psi_n \rangle = \sum_m \langle n | x^2 | m \rangle \langle m | x^2 | n \rangle$$

The left term expands as follows.

$$\begin{aligned} \langle n | x^2 | m \rangle &= \frac{\hbar}{2m\omega} \langle n | (a_+ + a_-)^2 | m \rangle \\ &= \frac{\hbar}{2m\omega} [\langle n | a_+^2 | m \rangle + \langle n | a_-^2 | m \rangle + 2 \langle n | a_+ a_- | m \rangle + \langle n | 1 | m \rangle] \\ &= \frac{\hbar}{2m\omega} [\sqrt{(m+1)(m+2)} \langle n | m+2 \rangle + \sqrt{m(m-1)} \langle n | m-2 \rangle + (2m+1) \langle n | m \rangle] \\ &= \frac{\hbar}{2m\omega} [\sqrt{(m+1)(m+2)} \delta_{n,m+2} + \sqrt{m(m-1)} \delta_{n,m-2} + (2m+1) \delta_{n,m}] \end{aligned}$$

Analogously, the right term expands to

$$\langle m | x^2 | n \rangle = \frac{\hbar}{2m\omega} [\sqrt{(n+1)(n+2)} \delta_{m,n+2} + \sqrt{n(n-1)} \delta_{m,n-2} + (2n+1) \delta_{m,n}]$$

Now since

$$(\delta_{n,m+2} + \delta_{n,m-2} + \delta_{n,m})(\delta_{m,n+2} + \delta_{m,n-2} + \delta_{m,n}) = \delta_{n,m+2} \delta_{m,n-2} + \delta_{n,m} \delta_{m,n} + \delta_{n,m-2} \delta_{m,n+2}$$

we have that

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

When  $m = n - 2$ , the first term will be nonzero. When  $m = n$ , the second term will be nonzero. And when  $m = n + 2$ , the third term will be nonzero. Taken together, this means that

$$\begin{aligned} \langle \psi_n | x^4 | \psi_n \rangle &= \frac{\hbar^2}{4m^2\omega^2} [\sqrt{(n-1)n} \sqrt{n(n-1)} \\ &\quad + (2n+1)(2n+1) + \sqrt{(n+2)(n+1)} \sqrt{(n+1)(n+2)}] \\ &= \frac{\hbar^2}{4m^2\omega^2} [n(n-1) + (2n+1)^2 + (n+1)(n+2)] \\ &= \frac{\hbar^2}{4m^2\omega^2} (6n^2 + 6n + 3) \end{aligned}$$

□

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

$$\sum_m |m\rangle \langle m| = I \quad (4.11)$$

and

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

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

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

Additionally, demonstrate numerically that — as expected — it always moves with a classical frequency  $\omega$  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.,

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

*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.

## 5 Three Dimensional Mathematical Tools

- 2/17: 1. Consider a three-dimensional box, such that the potential is given by

$$V(x, y, z) = V_1\theta(|x| - a) + V_2\theta(|y| - b) + V_3\theta(|z| - c) \quad (5.1)$$

where the function  $\theta$  is such that

$$\theta(u) = \begin{cases} 1 & u \geq 0 \\ 0 & u < 0 \end{cases} \quad (5.2)$$

This means that the potential is zero inside the box that extends from  $x = -a$  to  $x = a$  in the  $x$ -direction,  $y = -b$  to  $y = b$  in the  $y$ -direction, and  $z = -c$  to  $z = c$  in the  $z$ -direction and increases in steps otherwise.

- Analyze first the case wherein all of  $V_1, V_2, V_3 \rightarrow \infty$ . This is the infinite square well in three dimensions. What is the general solution for  $\psi(x, y, z)$ ? *Hint*: Use the method of separation of variables and write  $\psi(x, y, z) = X(x)Y(y)Z(z)$ .
  - Give an expression for the total energy of the system in terms of the energies associated with the propagation in the three space directions.
  - What happens when one of the three  $V_i$ 's becomes finite? What would be the possible solutions in such a case?
  - What happens when the three  $V_i$ 's become finite?
2. In the presence of a central force, the potential depends only on the radial distance and not on the direction, i.e.,

$$V(\vec{r}) = V(\sqrt{x^2 + y^2 + z^2}) \quad (5.3)$$

- Show that in such a potential, the momentum is not conserved (that is, its mean value is not independent of time), but the angular momentum  $\vec{L} = \vec{r} \times \vec{p}$  is conserved. *Hint*: Use commutation relations with  $\hat{H}$ . Test this for each component of  $\vec{L}$  separately.
- What happens if the system has a translational invariance in the  $z$ -direction and

$$V(\vec{r}) = V(\sqrt{x^2 + y^2}) \quad (5.4)$$

for all  $z$ ? Is any component of the momentum or angular momentum preserved?

- For part (b), what would be the mean value  $\langle \hat{z} \rangle(t)$  of the  $z$ -coordinate if the mean value  $\langle \hat{p}_z \rangle$  of the momentum in the  $z$ -direction is constant at  $p_0$  while  $\langle \hat{z} \rangle = 0$  at time  $t = 0$ ?
3. Imagine I have a potential such that I can find simultaneous eigenstates of  $\hat{L}^2$ ,  $\hat{L}_z$ , and  $\hat{H}$  with respective eigenvalues  $\hbar^2\ell(\ell+1)$ ,  $\hbar m$ , and  $E_{n\ell}$ . Suppose that  $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$ ,  $[\hat{L}^2, \hat{L}_i] = [\hat{H}, \hat{L}_i] = 0$ , and  $\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$ .

- Show that  $[\hat{L}_{\pm}, \hat{L}_z] = \mp\hbar\hat{L}_{\pm}$ .
- Show also that this implies that, given an eigenfunction  $Y_{\ell m}$  of  $\hat{L}^2$  and  $\hat{L}_z$ ,

$$\hat{L}_{\pm}Y_{\ell m} \propto Y_{\ell(m\pm 1)} \quad (5.5)$$

- Show that  $\hat{L}^2 = \hat{L}_- \hat{L}_+ + \hbar\hat{L}_z + \hat{L}_z^2$ .
- With the above information, use the ladder operators  $\hat{L}_{\pm}$  to compute the mean value of  $\hat{L}_z$ ,  $\hat{L}_y$ ,  $\hat{L}_x^2$ , and  $\hat{L}_y^2$  in an eigenstate of  $\hat{L}^2$  and  $\hat{L}_z$ .
- Discuss the uncertainty principle for the incompatible variables  $\hat{L}_x$  and  $\hat{L}_y$ . In which way does this differ from the case of  $\hat{x}$  and  $\hat{p}_x$ ?