PHY356 Problem Set 2 — Due Tuesday October 11, 2022

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9. Let H be the Hamiltonian operator of a physical system. Denote by $|\varphi_n\rangle$ the eigenvectors of H, with eigenvalues E_n:

$$H|\varphi_n\rangle = E_n|\varphi_n\rangle$$

a. For an arbitrary operator A, prove the relation:

$$\langle\varphi_n|[A,\, H]|\varphi_n\rangle = 0$$

b. Consider a one-dimensional problem, where the physical system is a particle of mass m with potential energy $V(X)$. In this case, H is written:

$$H = \frac{1}{2m}P^2 + V(X)$$

α. In terms of P, X and $V(X)$, find the commutators: $[H,\, P]$, $[H,\, X]$ and $[H, XP]$.

β. Show that the matrix element $\langle\varphi_n|P|\varphi_n\rangle$ (which we shall interpret in Chapter III as the mean value of the momentum in the state $|\varphi_n\rangle$) is zero.

γ. Establish a relation between $E_k = \langle\varphi_n|\dfrac{P^2}{2m}|\varphi_n\rangle$ (the mean value of the kinetic energy in the state $|\varphi_n\rangle$) and $\langle\varphi_n|X\dfrac{\mathrm{d}V}{\mathrm{d}X}|\varphi_n\rangle$. Since the mean value of the potential energy in the state $|\varphi_n\rangle$ is $\langle\varphi_n|V(x)|\varphi_n\rangle$, how is it related to the mean value of the kinetic energy when:

$$V(X) = V_0\, X^s$$

$(s = 2, 4, 6\, ...;\ V_0 > 0)$?

(a) I wish to show that for any arbitrary operator $\hat{A}$, that $\langle\varphi_n|\, [\hat{A},\, \hat{H}]\, |\varphi_n\rangle = 0$, where $|\varphi_n\rangle$ represents an eigenvector of the enrgy eigenvalue equation $\hat{H}\,|\varphi_n\rangle = E_n\,|\varphi_n\rangle$. We have that

$$\begin{aligned}
\langle\varphi_n|\, [\hat{A},\, \hat{H}]\, |\varphi_n\rangle &= \langle\varphi_n|\, \hat{A}\hat{H} - \hat{H}\hat{A}\, |\varphi_n\rangle && \text{(by commutator definition)}\\
&= \langle\varphi_n|\, \hat{A}\hat{H}\, |\varphi_n\rangle - \langle\varphi_n|\, \hat{H}\hat{A}\, |\varphi_n\rangle && \text{(by linearity)}\\
&= \langle\varphi_n|\, \hat{A}E_n\, |\varphi_n\rangle - \langle\varphi_n|\, \hat{H}\hat{A}\, |\varphi_n\rangle && \text{(by the energy eigenvalue equation)}\\
&= \langle\varphi_n|\, \hat{A}E_n\, |\varphi_n\rangle - \langle\varphi_n|\, \hat{H}^\dagger\hat{A}\, |\varphi_n\rangle && \text{(since Hamiltonian is Hermitian)}\\
&= E_n\, \langle\varphi_n|\, \hat{A}\, |\varphi_n\rangle - E_n\, \langle\varphi_n|\, \hat{A}\, |\varphi_n\rangle && \text{(by linearity)}\\
&= 0.
\end{aligned}$$

This implies that the expected value of any operator in commutation with the Hamiltonian is zero, which is what I wanted to show.

(b - α) To proceed, I will determine the following commutators: $[\hat{H},\hat{P}]$, $[\hat{H},\hat{X}]$, and $[\hat{H},\hat{X}\hat{P}]$:

$$\begin{aligned}
[\hat{H},\hat{P}] &= \left[\frac{\hat{P}^2}{2m}+V(\hat{X}),\hat{P}\right] \\
&= \frac{1}{2m}[\hat{P}^2,\hat{P}]+[V(\hat{X}),\hat{P}] \\
&= \frac{1}{2m}\left(\hat{P}[\hat{P},\hat{P}]+[\hat{P},\hat{P}]\hat{P}\right)+\left(V(\hat{X})\hat{P}-\hat{P}V(\hat{X})\right) \\
&= \frac{1}{2m}\left(\hat{P}(0)+(0)\hat{P}\right)\left(-i\hbar V(\hat{X})\frac{\partial}{\partial X}[1]+i\hbar\frac{\partial}{\partial X}[V(\hat{X})]\right) \\
&= i\hbar\frac{\partial V}{\partial x}
\end{aligned}$$

since the derivative of a constant is zero. For the next,

$$\begin{aligned}
[\hat{H},\hat{X}] &= \left[\frac{\hat{P}^2}{2m}+V(\hat{X}),\hat{X}\right] \\
&= \frac{1}{2m}[\hat{P}^2,\hat{X}]+[V(\hat{X}),\hat{X}] \\
&= \frac{1}{2m}\left(\hat{P}[\hat{P},\hat{X}]+[\hat{P},\hat{X}]\hat{P}\right)+\left(V(\hat{X})\hat{X}-]\hat{X}V(\hat{X})\right) \\
&= \frac{1}{2m}\left(\hat{P}[-i\hbar]+[-i\hbar]\hat{P}\right)-(V(\hat{X})x-V(\hat{X})x) \\
&= -\frac{1}{m}\cdot i\hbar\hat{P}+0 \\
&= -i\hbar\frac{\hat{P}}{m}.
\end{aligned}$$

Lastly, we can impose the two previous commutation relations to determine the third:

$$\begin{aligned}
[\hat{H},\hat{X}\hat{P}] &= \hat{X}[\hat{H},\hat{P}]+[\hat{H},\hat{P}]\hat{X} \\
&= \hat{X}\left(i\hbar\frac{\partial V}{\partial X}\right)+\left(-i\hbar\frac{\hat{P}}{m}\right)\hat{P} \\
&= i\hbar\hat{X}\frac{\partial V}{\partial X}-i\hbar\frac{\hat{P}^2}{m} \\
&= i\hbar\left(\hat{X}\frac{\partial V}{\partial X}-\frac{\hat{P}^2}{m}\right).
\end{aligned}$$

(b - β) It follows now to show that the matrix element $\langle\varphi_n|\,\hat{P}\,|\varphi_n\rangle=0$, that is, the expected value of the momentum, is zero. Using question (a), we have that the average value of anything commuting with the Hamiltonian is zero:

$$\langle\varphi_n|\,[\hat{H},\hat{X}]\,|\varphi_n\rangle=0.$$

However, as determined by the commutator relation $[\hat{H},\hat{X}]=-i\hbar\frac{\hat{P}}{m}$, we have that

$$\langle\varphi_n|\,[\hat{H},\hat{X}]\,|\varphi_n\rangle=\langle\varphi_n|\left(-i\hbar\frac{\hat{P}}{m}\right)|\varphi_n\rangle=-\frac{i\hbar}{m}\langle\varphi_n|\,\hat{P}\,|\varphi_n\rangle=0,$$

and since $-\dfrac{i\hbar}{m} \neq 0$, then it must be that the matrix element $\langle \varphi_n | \hat{P} | \varphi_n \rangle = 0$.

(b - γ) Consider previously the commutator $[\hat{H}, \hat{X}\hat{P}]$. From question (a), it must be that the expected value of the commutation is zero because $\hat{X}\hat{P}$ can be considered as arbitrary:

$$\langle \varphi_n | [\hat{H}, \hat{X}\hat{P}] | \varphi_n \rangle = 0.$$

Yet, with regard to question (b-α), this commutator is exaclty

$$[\hat{H}, \hat{X}\hat{P}] = i\hbar \left(\frac{\partial V}{\partial X} - \frac{\hat{P}^2}{m} \right).$$

By linearity, this implies that

$$\langle \varphi_n | i\hbar \left(\hat{X} \frac{\partial V}{\partial X} - \frac{\hat{P}^2}{m} \right) | \varphi_n \rangle = 0 \implies \langle \varphi_n | \hat{X} \frac{\partial V}{\partial X} | \varphi_n \rangle = \langle \varphi_n | \frac{\hat{P}^2}{m} | \varphi_n \rangle .$$

This relationship is equivalently

$$2 \langle \varphi_n | \frac{\hat{P}^2}{2m} | \varphi_n \rangle = 2 \langle E_k \rangle = \langle \varphi_n | \hat{X} \frac{\partial V}{\partial X} | \varphi_n \rangle .$$

Summing over all stationary states n, we determine the *virial theorem*, relating the average kinetic energy to the potential energy:

$$2 \langle E_k \rangle = \sum_{n=1}^{\infty} \langle \varphi_n | \hat{X} \frac{\partial V}{\partial X} | \varphi_n \rangle .$$

Allow me to consider a specifc case of potential, when $V(X) = V_0 X^s$. The virial theorem directly states that $X \dfrac{\partial V}{\partial X} = Xs \cdot V_0 X^{s-1} = s \cdot V_0 X^s = sV(X)$. Therefore the average kinetic energy is related to the average potential energy by

$$2 \langle E_k \rangle = \sum_{n=1}^{\infty} \langle \varphi_n | sV(X) | \varphi_n \rangle = s \langle V \rangle .$$

This is a very pleasant relationship for this case of potentials. To consider now a harmonic oscillator, the degree of the potential is $s = 2$, thus we find that the average kinetic energy is directly related to the average potential energy by

$$\langle T \rangle = \langle V \rangle .$$

For a classical harmonic oscillator, we have that $\dfrac{1}{2} m v^2 = \dfrac{1}{2} k x^2$, so the velocity of the particle is directly related to its position with regard to the potential. This is what we would have expected, so the result agrees with the theorem.

3. **(15 points)** Let C_{op} denote an operator which changes a function into its complex conjugate:

$$C_{op}\psi(x) = \psi^*(x)$$

(Note: This is not a linear operator)

(a) Determine whether or not C_{op} is Hermitian.

(b) Determine all possible eigenvalues of C_{op}.

(c) Do the eigenfunctions of C_{op} form a complete set? Are they orthogonal? Explain your answers.

(d) Let $H_{op} = \frac{-h^2}{2m}\nabla^2 + V(x)$ be the hamiltonian of a particle in some real valued potential well $V(x)$. Evaluate the commutator $[H_{op}, C_{op}]$. Discuss the implication of your result concerning stationary states of H_{op}.

(a) I need to determine whether or not $\hat{C}$ is Hermitian. Consider the following expression in terms of the continuous-space integral representation of bras and kets:

$$\langle\varphi|\,\hat{C}\,|\psi\rangle = \int_{-\infty}^{+\infty} dx\,\varphi^*(x)\hat{C}\psi(x) = \int_{-\infty}^{+\infty} dx\,\psi^*(x)\hat{C}\varphi(x) = \langle\psi|\,\hat{C}\,|\varphi\rangle\,.$$

If these two expressions in fact differ, we attain a contradiction and henceforth $\hat{C}$ is not self-adjoint. Yet $\hat{C}$ acting on $\varphi(x)$ is $\varphi^*(x)$, and similarly $\hat{C}\psi(x) = \psi^*(x)$. This implies that

$$\int_{-\infty}^{+\infty} dx\,\varphi^*(x)\hat{C}\psi(x) = \int_{-\infty}^{+\infty} dx\,\varphi^*(x)\psi^*(x) = \int_{-\infty}^{+\infty} dx\,\psi^*(x)\varphi^*(x) = \int_{-\infty}^{+\infty} dx\,\psi^*(x)\hat{C}\varphi(x),$$

so the expressions are equal! Therefore since $\langle\varphi|\,\hat{C}\,|\psi\rangle = \langle\psi|\,\hat{C}\,|\varphi\rangle$, and $(\langle\psi|\,\hat{C}\,|\varphi\rangle)^* = \langle\varphi|\,\hat{C}^\dagger\,|\psi\rangle$, then this directly implies that $\hat{C} = \hat{C}^\dagger$. Therefore $\hat{C}$ is Hermitian.

(b) The eigenvalues of $\hat{C}$ are determined by any eigenfunction of $\hat{C}$. In most cases, for an arbitrary $\psi(x)$, $\psi(x) \neq \psi^*(x) = \hat{C}\psi(x)$, because $\psi(x)$ is complex. Consider now an entirely real wavefunction (such as a stationary state) $\varphi(x)$. Then, since $\mathbb{Im}(\varphi(x)) = 0$, we obtain $\hat{C}\varphi(x) = (1)\varphi(x)$, so $\varphi(x)$ is an eigenfunction of $\hat{C}$ with eigenvalue 1. Similarly, suppose we had an entirely complex wavefunction $\chi(x)$: then $\mathbb{Re}(\chi(x)) = 0$, so $\hat{C}\chi(x) = (-1)\chi(x)$, so $\chi(x)$ is an eigenfunction of $\hat{C}$ with eigenvalue -1 which is due to conjugation.
Now allow me consider a general case. An arbitrary wavefunction $\psi(x)$ both a real and complex components, and we can decompose $\psi(x)$ into these components:

$$\psi(x) = \mathbb{Re}(\psi(x)) + i\mathbb{Im}(\psi(x)).$$

In such a case, $\hat{C}$ acting on $\mathbb{Re}(\psi(x))$ yields eigenvalue 1 with eigenfunction $\mathbb{Re}(\psi(x))$, and $\mathbb{Im}(\psi(x))$ eigenvalue -1 with eigenfunction $\mathbb{Im}(\psi(x))$. We can conclude from this that $\hat{C}$ has eigenvalues ± 1.

(c) By the definition of the complex plane, these real and imaginary components of the wavefunction must be orthogonal. However for two wavefunction $\psi_1(x)$ and $\psi_2(x)$, it may not always be the case that the imaginary and real components are orthogonal (because they are different functions), as in: $\int_{\mathbb{R}} \mathbb{R}\mathrm{e}(\psi_1(x))\mathbb{I}\mathrm{m}(\psi_2(x)) \neq 0$ generally. The eigenfunctions form a complete set because any wavefunction can be composed from a linear combination of real and complex functions. For instance, consider the time-dependent evolution of the stationary states of the infinite square well problem. They are given by $\varphi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{iE_n t/\hbar}$, which have a real component $\mathbb{R}\mathrm{e}(\varphi_n(x,t)) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{E_n t}{\hbar}\right)$ which is an eigenfunction of $\hat{C}$ with eigenvalue 1, and imaginary component $\mathbb{I}\mathrm{m}(\varphi_n(x,t)) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{E_n t}{\hbar}\right)$ which is an eigenfunction of $\hat{C}$ with eigenvalue -1. When integrated across all time, these components are orthogonal to each other because of the orthogonality of sin and cos.

(d) I will now evaluate the commutator of $[\hat{H}, \hat{C}]$. We have:

$$\begin{aligned}
[\hat{H}, \hat{C}] &= \hat{H}\hat{C} - \hat{C}\hat{H} \\
&= \hat{H}\hat{C} - \hat{C}\left(\frac{\hat{P}^2}{2m} + V(\hat{X})\right) \\
&= \hat{H}\hat{C} - \left(\frac{\hat{P}^2}{2m} + V(\hat{X})\right) \\
&= \hat{H}\left(\hat{C}[1] - 1\right) \\
&= \hat{H}(1 - 1) \\
&= 0.
\end{aligned}$$

Physically, this means that the two operators share the same eigenfunctions. This is as expected. For stationary states of $\hat{H}$, they are given by entirely real wavefunctions when solving the energy eigenvalue equation $\hat{H}\varphi_n(x) = E_n\varphi_n(x)$. As previously shown, any real $\varphi_n(x)$ will be an eigenfunction of $\hat{C}$ with eigenvalue 1.

4. **(20 points)**. A particle is confined in a one-dimensional box of length L. The Hamiltonian operator for the system is

$$H_{op} = \frac{P_{op}^2}{2m} + V(x_{op})$$

where

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

(a) Compute the probability density $|\langle p|\psi_1\rangle|^2$ that the particle in its ground state $|\psi_1\rangle$ has a momentum between p and $p+dp$. Plot your result as a function of p and discuss it's physical meaning.

(b) The motion of a classical particle in a box is periodic with period $T = 2L/\nu$ where ν is the particle's speed. Stationary states, do not exhibit such periodicity. In order to describe classical motion we must consider a superposition of eigenstates. Consider a particle which is initially ($t = 0$) in the state:

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle + |\ \psi_2\rangle)$$

where $\langle x|\psi_n\rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$. The subsequent time evolution of this state is given by

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle\, e^{-iE_1 t/h} + |\psi_2\rangle\, e^{-iE_2 t/h}$$

where E_1 and E_2 are the eigenvalues of the ground and first excited states. Calculate $\langle H_{op}\rangle$, $\langle x_{op}\rangle$ and $\langle p_{op}\rangle$ where we define $\langle A\rangle \equiv \langle\psi(t)|A|\psi(t)\rangle$ Plot your results as a function of time t. Show that $m\frac{d}{dt}\langle x_{op}\rangle = \langle p_{op}\rangle$ as you would expect classically.

(a) To determine the probability density $|\langle p|\psi_1\rangle|^2$, I can first determine the expression for the ground state wave in momentum space. By inserting the identity operator $|x\rangle\langle x| = \mathbb{1}$ into the inner product of the ground state with momentum, we obtain the expression for the Fourier Transform of $\psi_1(x)$ into momentum space:

$$\langle p|x\rangle\langle x|\psi\rangle = \sqrt{2\pi\hbar}\, e^{-ipx/\hbar}\langle p|\psi\rangle \implies \widetilde{\psi}(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx\, \psi(x,t) e^{-ipx/\hbar}.$$

Since we are examining the ground stationary state, $\psi_1(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) e^{-iE_1 t/\hbar}$, we should only integrate from 0 to L, since that is where the wavefunction is defined. It is zero outside of this region, hence $\tilde{\psi(p)}$ will also be zero. We have that

$$\widetilde{\psi}_1(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2}{L}} \int_0^L dx\, \sin\left(\frac{\pi x}{L}\right) e^{-ipx/\hbar} e^{-iE_1 t/\hbar}$$

$$= \frac{1}{\sqrt{\pi\hbar L}} e^{-iE_1 t/\hbar} \int_0^L dx\, \sin\left(\frac{\pi x}{L}\right) e^{-ipx/\hbar}.$$

Since any $\sin x$ can be expressed in terms of complex exponentials, $\sin x = \dfrac{e^{ix} - e^{-ix}}{2i}$, then

$$\begin{aligned}
\widetilde{\psi}_1(p,t) &= \frac{1}{2i\sqrt{\pi\hbar L}} e^{-iE_1 t/\hbar} \int_0^L dx\, [e^{i\pi x/L} - e^{-i\pi x/L}] e^{-ipx/\hbar} \\
&= \frac{1}{2i\sqrt{\pi\hbar L}} e^{-iE_1 t/\hbar} \int_0^L dx\, \exp\left[ix\left(\frac{\pi}{L} - \frac{p}{\hbar}\right)\right] - \exp\left[-ix\left(\frac{\pi}{L} + \frac{p}{\hbar}\right)\right].
\end{aligned}$$

This is not a difficult integral to compute:

$$\begin{aligned}
\widetilde{\psi}_1(p,t) &= \frac{1}{2i\sqrt{\pi\hbar L}} e^{-iE_1 t/\hbar} \left[\frac{1}{i\left(\frac{\pi}{L} - \frac{p}{\hbar}\right)} \exp\left[ix\left(\frac{\pi}{L} - \frac{p}{\hbar}\right)\right] + \frac{1}{i\left(\frac{\pi}{L} + \frac{p}{\hbar}\right)} \exp\left[-ix\left(\frac{\pi}{L} + \frac{p}{\hbar}\right)\right]\right]_0^L \\
&= \frac{1}{2i\sqrt{\pi\hbar L}} e^{-iE_1 t/\hbar} \left[\frac{1}{i\left(\frac{\pi}{L} - \frac{p}{\hbar}\right)} \exp\left[iL\left(\frac{\pi}{L} - \frac{p}{\hbar}\right)\right] + \frac{1}{i\left(\frac{\pi}{L} + \frac{p}{\hbar}\right)} \exp\left[-iL\left(\frac{\pi}{L} + \frac{p}{\hbar}\right)\right]\right] \\
&\qquad - \left[\left[\frac{1}{i\left(\frac{\pi}{L} - \frac{p}{\hbar}\right)} + \frac{1}{i\left(\frac{\pi}{L} + \frac{p}{\hbar}\right)}\right]\right].
\end{aligned}$$

We can now move forward into simplifying the expression. Factoring out a $\hbar L$, and distributing the L is the exponentials, we have

$$\widetilde{\psi}_1(p,t) = -\frac{\hbar L}{2\sqrt{\pi\hbar L}} \frac{e^{-iE_1 t/\hbar}}{\pi^2\hbar^2 - p^2L^2} \left[\left(e^{i(\pi - pL/\hbar)} - 1\right)(\pi\hbar + pL) + \left(e^{i(\pi + pL/\hbar)} - 1\right)(\pi\hbar - pL)\right].$$

When expanded, like terms can be collected. By the properties of the exponential exponentials, $e^{i\pi} = -1$ and thus can be factored and multiplied through:

$$\begin{aligned}
\widetilde{\psi}_1(p,t) &= -\frac{\hbar L}{2\sqrt{\pi\hbar L}} \frac{e^{-iE_1 t/\hbar}}{\pi^2\hbar^2 - p^2L^2} \left[\pi\hbar\left(e^{i\pi}e^{-pL/\hbar} + e^{-i\pi}e^{-pL/\hbar}\right) + pL\left(e^{i\pi}e^{-pL/\hbar} - e^{-i\pi}e^{-pL/\hbar}\right) - 2\pi\hbar\right] \\
&= -\frac{\hbar L}{2\sqrt{\pi\hbar L}} \frac{e^{-iE_1 t/\hbar}}{\pi^2\hbar^2 - p^2L^2} \left[\pi\hbar\left(-e^{-pL/\hbar} - e^{-pL/\hbar}\right) + pL\left(-e^{-pL/\hbar} + e^{-pL/\hbar}\right) - 2\pi\hbar\right] \\
&= -\frac{\hbar L}{2\sqrt{\pi\hbar L}} \frac{e^{-iE_1 t/\hbar}}{\pi^2\hbar^2 - p^2L^2} \left[-2\pi\hbar e^{-ipL/\hbar} - 2\pi\hbar + pL(0)\right]
\end{aligned}$$

Simplifying further the leading coefficient terms and factoring out a $\hbar^2$ from the denominator in the difference term, we finally obtain

$$\widetilde{\psi}_1(p,t) = \sqrt{\frac{\pi L}{\hbar}} \frac{1}{\pi^2 - \frac{p^2L^2}{\hbar^2}} \left(e^{-ipL/\hbar} + 1\right) e^{-iE_1 t/\hbar}.$$

However, this still can be simplified further! Consider the term $e^{-ipL/\hbar} + 1$. By Euler's theorem, this is equal to $\cos\left(\dfrac{pL}{\hbar}\right) - i\sin\left(\dfrac{pL}{\hbar}\right) + 1$. Now, $\cos(2x) = 2\cos^2 x - 1$ and $\sin(2x) = 2\sin x\cos x$, thus by factoring out a 2 in the argument of the complex exponential, we find that

$$\cos\left(2\cdot\frac{pL}{2\hbar}\right) - i\sin\left(2\cdot\frac{pL}{2\hbar}\right) + 1 = 2\cos^2\left(\frac{pL}{2\hbar}\right) - 1 - 2i\sin\left(\frac{pL}{2\hbar}\right)\cos\left(\frac{pL}{2\hbar}\right) + 1$$

$$
\begin{aligned}
&= 2\cos\left(\frac{pL}{2\hbar}\right)\left[\cos\left(\frac{pL}{2\hbar}\right) - i\sin\left(\frac{pL}{2\hbar}\right)\right] \\
&= 2\cos\left(\frac{pL}{2\hbar}\right) e^{-ipL/2\hbar}.
\end{aligned}
$$

Now plugging this expression into our above expression for $\widetilde{\psi}_1(p,t)$, and simplifying, we have that

$$
\widetilde{\psi}_1(p,t) = \sqrt{\frac{\pi L}{\hbar}} \frac{2}{\pi^2 - \frac{p^2L^2}{\hbar^2}} \cos\left(\frac{pL}{2\hbar}\right) e^{-ipL/2\hbar} e^{-iE_1t/\hbar}.
$$

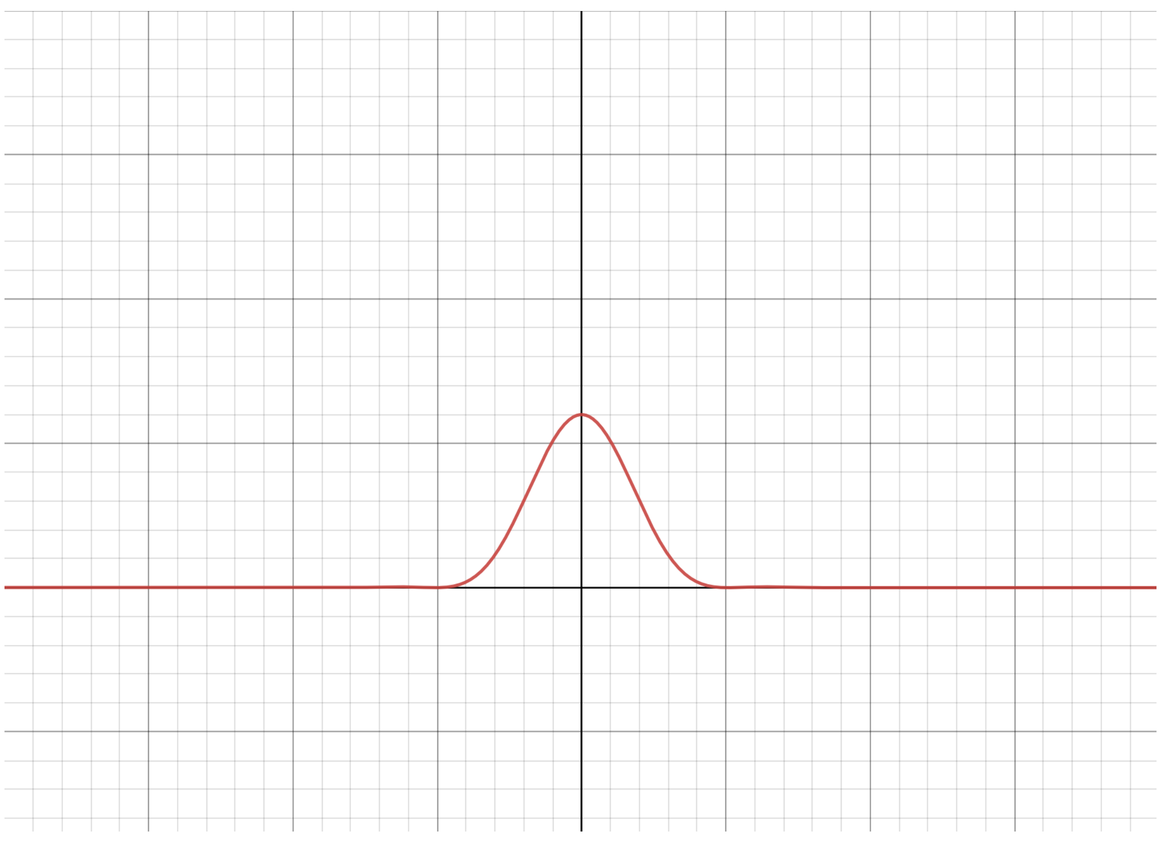
Both complex exponentials have complex modulus magnitude 1, thus they vanish when taking the complex square. Therefore

$$
\begin{aligned}
|\langle p|\psi_1\rangle|^2 = |\widetilde{\psi}_1(p,t)|^2 &= \left|\sqrt{\frac{\pi L}{\hbar}} \frac{2}{\pi^2 - \frac{p^2L^2}{\hbar^2}} \cos\left(\frac{pL}{2\hbar}\right) e^{-ipL/2\hbar} e^{-iE_1t/\hbar}\right|^2 \\
&= \left|\sqrt{\frac{\pi L}{\hbar}} \frac{2}{\pi^2 - \frac{p^2L^2}{\hbar^2}} \cos\left(\frac{pL}{2\hbar}\right)\right|^2 \\
&= \frac{4\pi L}{(\pi^2\hbar^2 - p^2L^2)^2} \cos^2\left(\frac{pL}{2\hbar}\right).
\end{aligned}
$$

The probability of finding the particle with momentum p between p and $p + dp$ is then given by

$$
d\mathbb{P} = |\langle p|\psi_1\rangle|^2 \, dp = \frac{4\pi L}{(\pi^2\hbar^2 - p^2L^2)^2} \cos^2\left(\frac{pL}{2\hbar}\right) dp.
$$

Now, the probability density of a momentum measurement can be plotted as a function of p and $\mathbb{P}$. Taking an arbitrary value of L, the momentum probability density appears as



The physical interpretation of this probability density is that the particle is most likely to have a momentum zero, but may have other values of momentum which are not zero. The reason the probability density is symmetric about the $p = 0$ axis is because we are not able to determine whether the particle in the infinite square well is moving to the left or to the right. The Heisenberg uncertainty principle justifies why the ground state position wavefunction and momentum wavefunction appear similar. It is easy to check that the integral $\mathbb{P} = \int_{\mathbb{R}} dp \, \frac{4\pi L}{(\pi^2\hbar^2 - p^2L^2)^2} \cos^2\left(\frac{pL}{2\hbar}\right) = 1$ across all possible values of momentum evaluates to 1. By Parseval's theorem, this integral should already be normalized.

(b) To proceed I shall determine the average (or expectation) values $\langle \hat{H} \rangle$, $\langle \hat{X} \rangle$, and $\langle \hat{P} \rangle$. The average value of an operator is given by $\langle \psi(t) | \hat{A} | \psi(t) \rangle$, thus we can proceed by taking inner products of bras and kets. When necessary, I shall turn to a continuous distribution expression of the inner product in which I can apply an integral. For the Hamiltonian, we have that

$$\begin{aligned}
\langle \hat{H} \rangle &= \langle \psi(t) | \hat{H} | \psi(t) \rangle \\
&= \frac{1}{\sqrt{2}} \left(\langle \psi_1 | e^{iE_1t/\hbar} + \langle \psi_2 | e^{iE_2t/\hbar} \right) \hat{H} \frac{1}{\sqrt{2}} \left(|\psi_1\rangle e^{-iE_1t/\hbar} + |\psi_2\rangle e^{-iE_2t/\hbar} \right) \\
&= \frac{1}{2} \left(\langle \psi_1 | e^{iE_1t/\hbar} + \langle \psi_2 | e^{iE_2t/\hbar} \right) \left[\hat{H} |\psi_1\rangle e^{-iE_1t/\hbar} + \hat{H} |\psi_2\rangle e^{-iE_2t/\hbar} \right] \\
&= \frac{1}{2} \left(\langle \psi_1 | e^{iE_1t/\hbar} + \langle \psi_2 | e^{iE_2t/\hbar} \right) \left(E_1 |\psi_1\rangle e^{-iE_1t/\hbar} + E_2 |\psi_2\rangle e^{-iE_2t/\hbar} \right) \\
&= \frac{1}{2} \Big(E_1 \langle \psi_1 | \psi_1 \rangle e^{iE_1t/\hbar} e^{-iE_1t/\hbar} + E_2 \langle \psi_1 | \psi_2 \rangle e^{iE_1t/\hbar} e^{-iE_2t/\hbar} \\
&\qquad + E_1 \langle \psi_2 | \psi_1 \rangle e^{iE_2t/\hbar} e^{-iE_1t/\hbar} + E_2 \langle \psi_2 | \psi_2 \rangle e^{iE_2t/\hbar} e^{-iE_2t/\hbar} \Big)
\end{aligned}$$

However, by the orthogonality of the eigenfunctions of the Hamiltonian operator, we have that $\langle \psi_i | \psi_j \rangle = 0$ for $i \neq j$, and $\langle \psi_i | \psi_j \rangle = 1$ for $i = j$, thus

$$\begin{aligned}
\langle \hat{H} \rangle &= \frac{1}{2} \left(E_1(1)(1) + E_2(0)e^{i(E_2 - E_1)t/\hbar} + E_1(0)e^{i(E_2 - E_1)t/\hbar} + E_2(1)(1) \right) \\
&= \frac{1}{2}(E_1 + E_2).
\end{aligned}$$

This is as expected, since the state is a linear combination of the two energies E_1, E_2. To determine $\langle \hat{X} \rangle$, I will move to an integral expression. The $i - th$ stationary state is given by $\psi_i(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{i\pi x}{L}\right) e^{-iE_it/\hbar}$. Therefore

$$\begin{aligned}
\langle \hat{X} \rangle &= \langle \psi(t) | \hat{X} | \psi(t) \rangle \\
&= \frac{1}{2} \int_0^L dx \left(\sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) e^{iE_1t/\hbar} + \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) e^{iE_2t/\hbar} \right) \\
&\qquad x \left(\sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) e^{-iE_1t/\hbar} + \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right) e^{-iE_2t/\hbar} \right) \\
&= \frac{1}{L} \int_0^L dx \left(\sin\left(\frac{\pi x}{L}\right) e^{iE_1t/\hbar} + \sin\left(\frac{2\pi x}{L}\right) e^{iE_2t/\hbar} \right) \\
&\qquad \left(x \sin\left(\frac{\pi x}{L}\right) e^{-iE_1t/\hbar} + x \sin\left(\frac{2\pi x}{L}\right) e^{-iE_2t/\hbar} \right)
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{L}\int_0^L dx\, \left(x\sin^2\left(\frac{\pi x}{L}\right) + x\sin^2\left(\frac{2\pi x}{L}\right) + x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) e^{i(E_2-E_1)t/\hbar} \right. \\
&\qquad\qquad \left. + x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) e^{-i(E_2-E_1)t/\hbar} \right) \\
&= \frac{1}{L}\int_0^L dx\, \left(x\sin^2\left(\frac{\pi x}{L}\right) + x\sin^2\left(\frac{2\pi x}{L}\right) \right. \\
&\qquad\qquad \left. + \left[e^{i(E_2-E_1)t/\hbar} + e^{-i(E_2-E_1)t/\hbar} \right] x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) \right),
\end{aligned}
$$

which all follows from distributing the brackets and collecting like terms. By the linearity of the integral, each term can be integrated separately then added back together. It is important to note that although these integrands appear similar to that of the Fourier orthogonality relations for sine and cosine, they are not zero over the bound of the period of the wave. This is due to the 'x' being multiplied through, making the integrand now an antisymmetric (odd) function. As a brief aside, I will evaluate each term. For lengths sake, I have applied integral calculator in places where I integration by parts could have been invoked. For generality, consider:

$$
\begin{aligned}
\int_0^L dx\, x\sin^2\left(\frac{n\pi x}{L}\right) &= \int_0^L dx\, \frac{x}{2}\left[1 - \cos\left(\frac{2n\pi x}{L}\right)\right] \\
&= \int_0^L dx\, \frac{x}{2} - \frac{x}{2}\cos\left(\frac{2n\pi x}{L}\right) \\
&= \frac{L^2}{4} - \frac{1}{2}\int_0^L dx\, x\cos\left(\frac{2n\pi x}{L}\right) \\
&= \frac{L^2}{4} + \frac{L^2}{4\pi^2 n^2}\left[2\pi n\sin(2\pi n) + \cos(2\pi n) - 1\right]. \qquad \text{(by integral calculator)}
\end{aligned}
$$

The second term is zero because it is an odd function for any $n \in \mathbb{Z}$. For the other integrand,

$$
\begin{aligned}
\int_0^L dx\, x\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) &= \int_0^L dx\, \frac{x}{2}\left[\cos\left(\frac{\pi x}{L} - \frac{2\pi x}{L}\right) - \cos\left(\frac{\pi x}{L} + \frac{2\pi x}{L}\right)\right] \\
&= \int_0^L dx\, \frac{x}{2}\left[\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right] \\
&= -\frac{1}{2}\left[\frac{2L^2}{\pi^2} - \frac{2L^2}{9\pi^2}\right] \qquad \text{(by integral calculator)} \\
&= -\frac{8L^2}{9\pi^2}.
\end{aligned}
$$

Therefore, collecting the terms, we have that

$$
\begin{aligned}
\langle \hat{X} \rangle &= \frac{1}{L}\left[\frac{L^2}{4} + \frac{L^2}{4} - \frac{8L^2}{9\pi^2}\left(e^{i(E_2-E_1)t/\hbar} + e^{-i(E_2-E_1)t/\hbar}\right)\right] \\
&= \frac{L}{2} - \frac{8L}{9\pi^2}\left(\cos((E_2-E_1)t/\hbar) + i\sin((E_2-E_1)t/\hbar) + \cos((E_2-E_1)t/\hbar) - i\sin((E_2-E_1)t/\hbar)\right) \\
&= \frac{L}{2} - \frac{16L}{9\pi^2}\cos\left(\frac{E_2-E_1}{\hbar}t\right) \\
&= \frac{L}{2} - \frac{16L}{9\pi^2}\cos\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}t\right),
\end{aligned}
$$

which is the time-evolution of the average value of the position of the particle. The energy difference $E_1 - E_2$ is just given by the stationary state energy:

$$\cos(E_2 - E_1)t/\hbar = \cos\left[\frac{(2)^2\pi^2\hbar^2}{2mL^2} - \frac{(1)^2\pi^2\hbar^2}{2mL^2}\right]\frac{t}{\hbar} = \cos\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}t\right).$$

Physically, this represents that the particle is most likely to be found in the middle of the box, yet oscillates around $\frac{L}{2}$ as time progresses. We can apply a similar process to determine the expectation value of the momentum, whose operator is defined by the derivative $\hat{P} = -i\hbar\frac{\partial}{\partial x}$. The application of the momentum operator is most useful when imposed in a continuous distribution, since we can directly apply the derivative to $\psi(x)$.

$$\begin{aligned}
\langle\hat{P}\rangle &= \langle\psi(t)|\hat{P}|\psi(t)\rangle \\
&= \frac{1}{2}\int_0^L dx\, \left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)e^{iE_1t/\hbar} + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)e^{iE_2t/\hbar}\right) \\
&\qquad\qquad \cdot (-i\hbar)\frac{\partial}{\partial x}\left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar} + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)e^{-iE_2t/\hbar}\right) \\
&= -\frac{i\hbar}{L}\int_0^L dx\, \left(\sin\left(\frac{\pi x}{L}\right)e^{iE_1t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{iE_2t/\hbar}\right) \\
&\qquad\qquad \cdot \frac{\partial}{\partial x}\left(\sin\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{-iE_2t/\hbar}\right) \\
&= -\frac{i\hbar}{L}\int_0^L dx\, \left(\sin\left(\frac{\pi x}{L}\right)e^{iE_1t/\hbar} + \sin\left(\frac{2\pi x}{L}\right)e^{iE_2t/\hbar}\right) \\
&\qquad\qquad \cdot \left(\frac{\pi}{L}\cos\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar} + \frac{2\pi}{L}\cos\left(\frac{2\pi x}{L}\right)e^{-iE_2t/\hbar}\right) \\
&= -\frac{i\hbar}{L}\int_0^L dx\, \left[\frac{\pi}{L}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right) + \frac{2\pi}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right)\right. \\
&\qquad\qquad \left. + \frac{\pi}{L}\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)e^{-i(E_2-E_1)t/\hbar} + \frac{2\pi}{L}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right)e^{i(E_2-E_1)t/\hbar}\right].
\end{aligned}$$

By the Fourier orthogonality relations of sine and cosine, the first two terms integrate to zero (the arguments contain identicle frequencies). The second two terms are not zero because we are not integrating over a full period; the arguments contain different frequencies. These integrals are easy to compute via the sine and cosine multiplication identities, but once again for lengths sake I will apply integral calculator:

$$\begin{aligned}
\int_0^L dx\, \sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right) &= \frac{4L}{3\pi} \\
\int_0^L dx\, \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{2\pi x}{L}\right) &= -\frac{2L}{3\pi}. \qquad \text{(by integral calculator)}
\end{aligned}$$

Therefore we find that

$$\langle\hat{P}\rangle = -\frac{i\hbar}{L}\left[0 + 0 + \frac{\pi}{L}\frac{4L}{3\pi}e^{-i(E_2-E_1)t/\hbar} - \frac{2\pi}{L}\frac{2L}{3\pi}e^{i(E_2-E_1)t/\hbar}\right]$$

$$
\begin{aligned}
&= -i\hbar\left(\frac{4}{3L}e^{-i(E_2-E_1)t/\hbar} - \frac{4}{3L}e^{i(E_2-E_1)t/\hbar}\right)\\
&= -i\hbar\frac{4}{3L}\left[\cos\left(\frac{(E_2-E_1)t}{\hbar}\right) - i\sin\left(\frac{(E_2-E_1)t}{\hbar}\right) - \cos\left(\frac{(E_2-E_1)t}{\hbar}\right) - i\sin\left(\frac{(E_2-E_1)t}{\hbar}\right)\right]\\
&= -i^2\hbar\frac{8}{3L}\sin\left(\frac{(E_2-E_1)t}{\hbar}\right)\\
&= \frac{8\hbar}{3L}\sin\left(\frac{(E_2-E_1)t}{\hbar}\right).
\end{aligned}
$$

Again, by utilizing the energy difference

$$
\sin\left(\frac{(E_2-E_1)t}{\hbar}\right) = \sin\left(\frac{3\pi^2\hbar}{2mL^2}\,t\right),
$$

the momentum expectation value becomes

$$
\langle\hat{P}\rangle = \frac{8\hbar}{3L}\sin\left(\frac{3\pi^2\hbar}{2mL^2}\,t\right).
$$

Due to the classical relationship $m\dfrac{dx}{dt} = p$, we shall expect the same result classically. We have that

$$
\begin{aligned}
\frac{d\,\langle\hat{X}\rangle}{dt} &= \frac{d}{dt}\left[\frac{L}{2} - \frac{16L}{9\pi^2}\cos\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}\,t\right)\right]\\
&= -\frac{16L}{9\pi^2}\frac{d}{dt}\cos\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}\,t\right)\\
&= \frac{16L}{9\pi^2}\sin\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}\,t\right)\cdot\frac{3}{2}\frac{\pi^2\hbar}{mL^2}\\
&= \frac{48}{18}\frac{\hbar}{mL}\sin\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}\,t\right)\\
&= \frac{1}{m}\cdot\frac{8\hbar}{3L}\sin\left(\frac{3}{2}\frac{\pi^2\hbar}{mL^2}\,t\right)\\
&= \frac{1}{m}\,\langle\hat{P}\rangle\,,
\end{aligned}
$$

which indeed suits the classical relationship. The values of $\langle\hat{H}\rangle\,,\langle\hat{X}\rangle$ and $\langle\hat{P}\rangle$ are all plotted below as a function of time for an arbitrary values of L,m and the energies: