1. (50 points) You have a particle of mass m confined to a 1D box between $-\frac{a}{2} < x < \frac{a}{2}$. Take the set of states $\{|n\rangle\}$ to refer to the eigenstates of the Hamiltonian; $\hat{H}|n\rangle = n^2 E_1 |n\rangle$, for $n = 1, 2, 3, \ldots$.

(a) What is $[\hat{H}, \hat{\mathcal{P}}]$, the commutator of the Hamiltonian and the parity?

Answer: As with other examples we did, if $V(x) = V(-x)$ and $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, then $[\hat{H}, \hat{\mathcal{P}}] = 0$. Both are true in this case, therefore the commutator is zero.

Since the energies are nondegenerate, this also means that every $\hat{H}$ eigenfunction is also a $\hat{\mathcal{P}}$ eigenfunction.

(b) Find the eigenfunctions $\langle x|n\rangle$.

Answer: These are just the wavefunctions that are the position representations of the Hamiltonian eigenvectors. We already know the solutions to the asymmetric well between 0 and L; all we need to get the new eigenfunctions is to change L to a and shift $x \to x - \frac{a}{2}$. The $+1$ parity solutions are $\varphi_n = \sqrt{\frac{2}{a}} \cos \frac{n\pi}{L} x$, for odd values of n. The -1 parity solutions are $\varphi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{L} x$, for even values of n.

Depending on how you construct these, you may get ± 1 multiplying your wavefunctions. This is just an overall phase; as long as you are consistent, it won't matter for any probabilities or expectation values. In the following, I will take the φ_n to just have a + sine or cosine in all cases.

(c) In the basis of energy eigenvectors, $\hat{x}$ and $\hat{p}$ are

$$\hat{x} = \sum_{mn} |m\rangle\langle m|\hat{x}|n\rangle\langle n| = \sum_{mn} x_{mn}|m\rangle\langle n|$$

where $x_{mn} = \langle m|\hat{x}|n\rangle$; and

$$\hat{p} = \sum_{mn} |m\rangle\langle m|\hat{p}|n\rangle\langle n| = \sum_{mn} p_{mn}|m\rangle\langle n|$$

where $p_{mn} = \langle m|\hat{p}|n\rangle$.

Find expressions for the matrix elements x_{mn} and p_{mn}, for arbitrary m and n. Simplify the expressions as much as possible (look up some trigonometric identities). Just to make it easy for me to check your answer, write down the a-dependent values for x_{mn} and p_{mn} for $m, n = 1, 2, 3, 4$ (the 4×4 sub-matrices).

Hint: Paying attention to parity will simplify many of your integrals.

Answer: Convert to wave function integrals:

$$\langle m|\hat{x}|n\rangle = \int dx\, \varphi_m^* \, x \, \varphi_n$$

If m and n are of the same parity, the integral will be zero, since x is an odd function. Also, since the φ_n are real, and $\langle m|\hat{x}|n\rangle = \langle n|\hat{x}|m\rangle^* = \langle n|\hat{x}|m\rangle$, this means $x_{mn} = x_{nm}$. So we only need do the integral for even n and odd m (or vice versa). In this case,

$$x_{nm} = \frac{2}{a}\int_{-a/2}^{a/2} dx\, x \,\sin\frac{n\pi}{a}x\,\cos\frac{m\pi}{a}x$$

After use of integral tables and some algebra,

$$x_{nm} = \frac{2a}{\pi^2}\left[\frac{1}{(n+m)^2} - \frac{1}{(n-m)^2}\right](-1)^{(n+m-1)/2}$$

The $\hat{p}$ matrix elements are also 0 for states of the same parity, since the derivative reverses parity. Now, however, $\langle m|\hat{p}|n\rangle = \langle n|\hat{p}|m\rangle^* = -\langle n|\hat{p}|m\rangle$; this means $p_{mn} = -p_{nm}$ because of $i^* = -i$. So we take n even and m odd again, with

$$p_{nm} = i\hbar\,\frac{2}{a}\int_{-a/2}^{a/2} dx\, \sin\frac{n\pi}{a}x\,\frac{\partial}{\partial x}\cos\frac{m\pi}{a}x$$

Again, after some algebra, the result is

$$p_{nm} = -\frac{4i\hbar}{a}\frac{nm}{(n^2-m^2)}(-1)^{(n+m-1)/2}$$

The first 4×4 submatrix for $\hat{x}$ is:

$$\frac{16a}{\pi^2}\begin{pmatrix} 0 & 1/9 & 0 & -2/225 \\ 1/9 & 0 & -3/25 & 0 \\ 0 & -3/25 & 0 & 6/49 \\ -2/225 & 0 & 6/49 & 0 \end{pmatrix}$$

For $\hat{p}$,

$$\frac{8i\hbar}{a}\begin{pmatrix} 0 & -1/3 & 0 & 2/15 \\ 1/3 & 0 & 3/5 & 0 \\ 0 & -3/5 & 0 & -6/7 \\ -2/15 & 0 & 6/7 & 0 \end{pmatrix}$$

(d) At $t = 0$, the particle is in an initial state

$$|\psi\rangle = \frac{1}{\sqrt{6}}\left(|1\rangle + |2\rangle - 2i|3\rangle\right)$$

Find the expectation value $\langle x\rangle$ as a function of time t. Your answers should have sine or cosine terms in it.

Answer: Putting in the time evolution,

$$\begin{aligned}\langle\psi|\hat{U}^{\dagger}(t)\,\hat{x}\,\hat{U}(t)|\psi\rangle &= \tfrac{1}{6}\quad\left(e^{i\omega_1 t}\langle 1| + e^{i\omega_2 t}\langle 2| + 2i\,e^{i\omega_3 t}\langle 3|\right)\hat{x} \\ &\qquad\left(e^{-i\omega_1 t}|1\rangle + e^{-i\omega_2 t}|2\rangle - 2i\,e^{-i\omega_3 t}|3\rangle\right)\end{aligned}$$

The only relevant non-zero matrix elements of $\hat{x}$ as calculated from part (a) are $x_{12} = x_{21}^*$ and $x_{23} = x_{32}^*$. Using these, we get

$$\langle x\rangle = \frac{8a}{3\pi^2}\left[\frac{1}{9}\left(e^{i(\omega_1-\omega_2)t} + e^{i(\omega_2-\omega_1)t}\right) - \frac{6i}{25}\left(e^{i(\omega_3-\omega_2)t} - e^{i(\omega_2-\omega_3)t}\right)\right]$$

Converting to cosines and sines, and using $\omega_n = n^2\,\omega_1$, we get

$$\langle x\rangle = \frac{8a}{3\pi^2}\left[\frac{2}{9}\cos 3\omega_1 t + \frac{12}{25}\sin 5\omega_1 t\right]$$

(e) Find $\langle p\rangle$ as a function of t when you start with the same initial state $|\psi\rangle$.

Answer: As in the previous case,

$$\begin{aligned}\langle\psi|\hat{U}^{\dagger}(t)\,\hat{p}\,\hat{U}(t)|\psi\rangle &= \tfrac{1}{6}\quad\left(e^{i\omega_1 t}\langle 1| + e^{i\omega_2 t}\langle 2| + 2i\,e^{i\omega_3 t}\langle 3|\right)\hat{p} \\ &\qquad\left(e^{-i\omega_1 t}|1\rangle + e^{-i\omega_2 t}|2\rangle - 2i\,e^{-i\omega_3 t}|3\rangle\right)\end{aligned}$$

We've computed the relevant $\hat{p}$ matrix elements in part (a). Putting them in gives

$$\langle p \rangle = \frac{4\hbar}{3a}\left[\frac{i}{3}\left(-e^{i(\omega_1-\omega_2)t}+e^{i(\omega_2-\omega_1)t}\right)-\frac{6}{5}\left(e^{i(\omega_3-\omega_2)t}+e^{i(\omega_2-\omega_3)t}\right)\right]$$

Which leads to

$$\langle p \rangle = \frac{4\hbar}{3a}\left[-\frac{2}{3}\sin 3\omega_1 t+\frac{12}{5}\cos 5\omega_1 t\right]$$

(f) Check whether

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

Is this a surprise? (Look up "Ehrenfest theorem.")

Answer: Using $\omega_1 = E_1/\hbar = \hbar\pi^2/2ma^2$, we find that

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

is correct. This is as we should expect, given the Ehrenfest theorem.

(g) Your initial state at $t = 0$ is again $|\psi\rangle$ from (d). Find the probability distribution for measurements of the parity $\mathcal{P}$ as a function of t.

Answer: States $|1\rangle$ and $|3\rangle$ have $+1$ parity; $|2\rangle$ has -1 parity. Clearly the time-dependent phases don't affect the probabilities, which are

$$P(+1) = \frac{1}{6}+\frac{4}{6}=\frac{5}{6} \qquad P(-1)=\frac{1}{6}$$

As it should be, since parity is conserved.

(h) Say that at a time $t > 0$, you measure an even parity for your particle with initial state $|\psi\rangle$ at $t = 0$. What is the new state $|\varphi\rangle$ immediately after the parity measurement?

Answer: Take the projection onto the even parity subspace, and re-normalize it:

$$|\varphi\rangle = \frac{1}{\sqrt{5}} \left(e^{-i\omega_1 t} |1\rangle - 2i\, e^{-i\omega_3 t} |3\rangle \right)$$