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**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  $n = 1, 2, 3, \dots$ . You already know the eigenfunctions  $\langle x|n\rangle$ .

(a) You can write the energy representations of the operators  $\hat{x}$  and  $\hat{p}$ , by saying

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

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  $4 \times 4$  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  $\varphi_n$  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  $4 \times 4$  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  $\hat{p}$ ,

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

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

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

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,

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

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

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

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

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

- (c) 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,

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

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

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

- (d) Check whether

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

Should this equality hold or not?

**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 Ehrenfest's Principle.

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- (e) Your initial state at  $t = 0$  is again  $|\psi\rangle$  from (b). Find the probability distribution for measurements of the parity as a function of  $t$ .

**Answer:** Write the state as a sum of *normalized* parity eigenstates:

$$\hat{U}(t)|\psi\rangle = \frac{\sqrt{5}}{\sqrt{6}} \left[ \frac{1}{\sqrt{5}} \left( e^{-i\omega_1 t} |1\rangle - 2i e^{-i\omega_3 t} |3\rangle \right) \right] + \frac{1}{\sqrt{6}} e^{-i\omega_2 t} |2\rangle$$

Clearly the time-dependent phases don't affect the probabilities, which are

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

As it should be, since parity is conserved.

- (f) 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:

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

2. (30 points) Starting from the following:

$$\langle x|x'\rangle = \delta(x-x') \quad , \quad \langle k|k'\rangle = \delta(k-k')$$

$$\int dx |x\rangle\langle x| = \hat{I} \quad , \quad \int dk |k\rangle\langle k| = \hat{I}$$

$$\hat{x} = \int dx x |x\rangle\langle x| \quad , \quad \hat{p} = \hbar \int dk k |k\rangle\langle k|$$

$$\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}}$$

Prove that

$$[\hat{x}, \hat{p}] = i\hbar$$

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*Hint:* Remember that

$$\frac{1}{2\pi} \int d\omega e^{i\omega(y-y')} = \delta(y-y') \quad \text{where} \quad \int dy \delta(y-z) f(y) = f(z)$$

$$\frac{1}{2\pi} \int d\omega \omega e^{i\omega(y-y')} = -i\delta'(y-y') \quad \text{where} \quad \int dy \delta'(y-z) f(y) = -f'(z)$$

**Answer:** We have

$$\hat{x}\hat{p} = \hbar \int dk dx x k |x\rangle\langle x|k\rangle\langle k| \quad \text{and} \quad \hat{p}\hat{x} = \hbar \int dx dk k x |k\rangle\langle k|x\rangle\langle x|$$

Let's try to make  $\hat{p}\hat{x}$  look more like  $\hat{x}\hat{p}$ . Therefore

$$\hat{p}\hat{x} = \hbar \int dx dk k x \frac{e^{-ikx}}{\sqrt{2\pi}} |k\rangle\langle x|$$

But we need to write the  $|k\rangle$  in terms of the  $|x\rangle$  vectors and vice versa. So,

$$|k\rangle = \int dx' |x'\rangle \langle x'|k\rangle = \int dx' \frac{e^{ikx'}}{\sqrt{2\pi}} |x'\rangle$$

$$\langle x| = \int dk' \langle x|k'\rangle \langle k'| = \int dk' \frac{e^{ik'x}}{\sqrt{2\pi}} \langle k'|$$

And therefore

$$\begin{aligned} \hat{p}\hat{x} &= \hbar(2\pi)^{-\frac{3}{2}} \int dx dk dx' dk' kx e^{-ikx} e^{ik'x} e^{ikx'} |x'\rangle\langle k'| \\ &= \hbar(2\pi)^{-\frac{1}{2}} \int dx dx' dk' x e^{ik'x} |x'\rangle\langle k'| \frac{1}{2\pi} \int dk k e^{ik(x'-x)} \\ &= \hbar(2\pi)^{-\frac{1}{2}} \int dx dx' dk' x e^{ik'x} |x'\rangle\langle k'| (-i)\delta'(x'-x) \\ &= -i\hbar(2\pi)^{-\frac{1}{2}} \int dx' dk' [e^{ik'x'} + ix'k' e^{ik'x'}] |x'\rangle\langle k'| \\ &= -i\hbar(2\pi)^{-\frac{1}{2}} \int dx' dk' e^{ik'x'} |x'\rangle\langle k'| + \hat{x}\hat{p} \\ &= -i\hbar \int dx' dk' |x'\rangle\langle x'|k'\rangle\langle k'| + \hat{x}\hat{p} \\ &= -i\hbar\hat{I}\hat{I} + \hat{x}\hat{p} \end{aligned}$$

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Therefore

$$[\hat{x}, \hat{p}] = i\hbar$$

**3. (20 points)** You have a free particle in 1D with an initial wave function  $\psi(x, 0)$ . Find an expression giving  $\langle \mathcal{P} \rangle$  as a function of time ( $\hat{\mathcal{P}}$  is the parity operator), and using this, directly confirm that  $\langle \mathcal{P} \rangle$  is conserved.

**Answer:** Expand  $\psi$  in terms of the  $e^{ikx}$  eigenfunctions for  $\hat{H}$ :

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

Therefore the time evolution is

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int dk e^{ikx} \phi(k) e^{-i\omega(k)t}$$

where  $\omega(k) = \hbar k^2 / 2m$ .

Now for the parity expectation:

$$\begin{aligned} \langle \mathcal{P} \rangle &= \int dx \psi^* \hat{\mathcal{P}} \psi = \int dx \psi^*(x, t) \psi(-x, t) \\ &= \frac{1}{2\pi} \int dx dk dk' e^{-ikx} \phi(k) e^{i\omega(k)t} e^{-ik'x} \phi(k') e^{-i\omega(k')t} \\ &= \int dk dk' \phi(k) e^{i\omega(k)t} \phi(k') e^{-i\omega(k')t} \frac{1}{2\pi} \int dx e^{-ix(k+k')} \\ &= \int dk dk' \phi(k) e^{i\omega(k)t} \phi(k') e^{-i\omega(k')t} \delta(-k - k') \\ &= \int dk \phi(k) e^{i\omega(k)t} \phi(-k) e^{-i\omega(-k)t} \end{aligned}$$

Now, notice that  $\omega(k) = \omega(-k)$ , therefore

$$\langle \mathcal{P} \rangle = \int dk \phi(k) \phi(-k)$$

which does not depend on time. Therefore  $\langle \mathcal{P} \rangle$  is conserved.