Physics 137A: Quantum Mechanics **Fall 2023**

PSET 05, Due October 12

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Problem 1:

1. We want to find the normalized position space wavefunction for a momentum eigenstate $\mid p\rangle$ i.e. we want to find $\langle x|p\rangle \equiv \psi_p(x)$.

   Since $\mid p\rangle$ is an eigenvector of the momentum operator $\hat{P}$, we have

   $$\hat{P} \mid p\rangle = p \mid p\rangle$$

   Now, we know how the momentum operator acts on a ket $\mid \psi\rangle$ in position space:

   $$\langle x|\hat{P}|\psi\rangle = -i\hbar\frac{d\psi}{dx}$$

   So, then, fro an eigenvector $\mid p\rangle$, we have $\langle x|\hat{P}|\psi\rangle = \langle x|(p|p\rangle) = p\langle x|p\rangle = p\psi_p(x)$

   $$p\psi_p = -i\hbar\frac{d\psi_p}{dx}$$

   Since we are dealing with just one variable, we can carry out a simple separation of variables to get

   $$\frac{ip}{\hbar}\int dx = \int \frac{d\psi_p}{\psi_p}$$

   (since $\frac{1}{(-i)} = i$) which gives us

   $$\begin{aligned}\frac{ip}{\hbar}x &= \ln(\psi_p) + C_1 \\ &= \ln C_0\psi_p\end{aligned}$$

   where $C_0 = \ln(C_1)$ So, exponentiating both sides, we obtain

   $$\psi_p = \frac{1}{C_0}e^{\frac{ipx}{\hbar}}$$

   But again, we can write $\frac{1}{C_0}$ more simply as some other constant C. So,

   $$\boxed{\psi_p(x) = \langle x|p\rangle = Ce^{\frac{ipx}{\hbar}}} \tag{5.1}$$

   We can find the constant C using the normalization condition $\langle p|p'\rangle = \delta(p - p')$ as

$$
\begin{aligned}
\langle p|p'\rangle &= \langle p|\mathbb{1}|p'\rangle \\
&= \int dx\ \langle p|x\rangle\langle x|p'\rangle \\
&= \int dx\ \langle x|p\rangle^*\langle x|p'\rangle \\
&= \int dx\ C^* e^{-\frac{ipx}{\hbar}} \cdot C e^{\frac{ipx}{\hbar}} \\
&= |C|^2 \int dx\ e^{i(p'-p)x/\hbar}
\end{aligned}
$$

To proceed, we use the following mathematical identity:

$$\int dk\ e^{ik(x-x')} = 2\pi\delta(x-x')$$

or, in the notation we will apply it to,

$$\boxed{\int dx\ e^{ik(p-p')} = 2\pi\delta(p-p')}$$

So, we have

$$
\begin{aligned}
\langle p|p'\rangle &= |C|^2 \int dx\ e^{i(p'-p)x/\hbar} \\
&= \hbar|C|^2 \int \left(\frac{dx}{\hbar}\right)\ e^{i\frac{x}{\hbar}(p-p')} \\
&= \hbar|C|^2 \cdot (2\pi\delta(p-p')) \\
&= (2\pi\hbar)\cdot |C|^2\delta(p-p')
\end{aligned}
$$

So,

$$\delta(p-p') = (2\pi\hbar)\cdot|C|^2\delta(p-p')$$

Thus, we obtain the result

$$|C| = \frac{1}{\sqrt{2\pi\hbar}}$$

By convention, we choose C to be a real number, so we simply have

$$C = \frac{1}{\sqrt{2\pi\hbar}}$$

Finally, the expression for the momentum wavefunction in position space is

$$\boxed{\langle x|p\rangle \equiv \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}}$$

2. Now, we want to find the matrix elements of the position operator in the momentum space. We know that in position space, the position operator looks like

$$\langle x|\hat{X}|x'\rangle = x\delta(x-x')$$

and we want to carry out a change of basis from the position eigenvectors to the momentum eigenvectors.

We can do this by kind of going in the opposite direction and starting off with $\langle p|\hat{X}|p'\rangle$ and inserting completenes i.e. $\mathbb{1} = \int dx \ \ | \, x\rangle\langle x \, |$

We have

$$\begin{aligned}
\langle p|\hat{X}|p'\rangle &= \langle p|\hat{X}|p'\rangle \\
&= \int dx \ \langle p|X|x\rangle\langle x|p'\rangle \\
&= \int dx \ x\langle p|x\rangle\langle x|p'\rangle \\
&= \int dx \ x\left(\frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}\right)\cdot\left(\frac{1}{\sqrt{2\pi\hbar}}e^{ip'x/\hbar}\right) \\
&= \frac{1}{2\pi\hbar}\int dx \ xe^{i\frac{x}{\hbar}(p'-p)} \\
&= \frac{1}{2\pi\hbar}\int dx \ (i\hbar)\cdot\left(\frac{d}{dp}e^{i\frac{x}{\hbar}(p-p)}\right) \\
&= \frac{i\hbar}{2\pi\hbar}\left(\frac{d}{dp}\int dx \ e^{i\frac{x}{\hbar}(p'-p)}\right)
\end{aligned}$$

Now, using the same identity we used in part(a), we know that

$$\int dx \ e^{i\frac{x}{\hbar}(p-p')} = \int dx \ e^{ix(\frac{p-p'}{\hbar})} = 2\pi\delta\left(\frac{p-p'}{\hbar}\right)$$

So, our postion operator in momentum space is

$$\begin{aligned}
\langle p|\hat{X}|p'\rangle &= \frac{i\hbar}{2\pi\hbar}\cdot\frac{d}{dp}\left(2\pi\delta\left(\frac{p-p'}{\hbar}\right)\right) \\
&= \frac{i\hbar}{2\pi\hbar}\cdot\frac{d}{dp}\left[2\pi\hbar\delta(p-p')\right] \\
&= i\hbar\frac{d}{dp}\delta(p-p')
\end{aligned}$$

So, the representation of our position operator in momentum space is

$$\boxed{\langle p|\hat{X}|p'\rangle = i\hbar\frac{d}{dp}\delta(p-p')}$$

This means that for a general state $| \, \psi\rangle$ we have

$$\langle p|\hat{X}|\psi\rangle = i\hbar\frac{d}{dp}\psi(p)$$

So, in position space, applying the Position operator looks like

$$\langle p|\hat{X}|\psi\rangle = \hat{\mathcal{X}}\psi(p)$$

where $\hat{\mathcal{X}} = i\hbar\frac{d}{dp}$ and $\psi(p) \equiv \langle p|\psi\rangle$

3. Now, we had originally *defined* the position operator $\hat{P}$ to be the generator of spatial translations. i.e.

$$e^{iaP/\hbar} \mid x\rangle = \mid x+a\rangle$$

And considering a to be some infinitessimal translation ϵ, we found that $\hat{P}$ in position space could be expressed as

$$\langle x|\hat{P}|x'\rangle = -i\hbar\frac{d}{dx}\delta(x-x')$$

or

$$\langle x|\hat{P}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x)$$

We found a VERY similar expression for the *postiion operator* in *momentum space* as

$$\langle p|\hat{X}|\psi\rangle = i\hbar\frac{d}{dp}\psi(p)$$

This suggests to us that the position operator plays a similar role in momentum space i.e. **The postiion operator is the generator of momentum translation.**

Problem 2:

1. Suppose we have two states $\mid \psi_1\rangle$ and $\mid \psi_2\rangle$. Then, we can shift into the position space to express their inner product as

$$\begin{aligned}\langle\psi_2|\psi_1\rangle &= \int dx\ \langle\psi_2|x\rangle\langle x|\psi_1\rangle \\ &= \int dx\ \langle x|\psi_2\rangle^*\langle x|\psi_1\rangle \\ &= \int dx\ \psi_2(x)^*\psi_1(x)\end{aligned}$$

Therefore,

$$\boxed{\langle\psi_2|\psi_1\rangle = \int dx\ \psi_2(x)^*\psi_1(x)}$$

2. A state $\mid \psi\rangle$ is normalized if $\langle\psi|\psi\rangle = 1$. Using part (a), we have

$$\langle\psi|\psi\rangle = \int dx\ \psi(x)^*\psi(x)$$

But, since $\psi(x)$ is just some complex number, we know that $\psi(x)^*\psi(x) = |\psi(x)|^2$

Thus, in the position basis, the normalization condition looks like

$$\boxed{\int dx\ |\psi(x)|^2 = 1}$$

3. We know that, in position space, the position operator $\hat{X}$ acts on a state $\mid \psi\rangle$ by multiplying the (position-space) wavefunction with x. That is,

$$\hat{X} \mid \psi\rangle \rightarrow x\psi(x)$$

Now, the expectation value for the operator is found as

$$\begin{aligned}\langle\psi|\hat{X}|\psi\rangle &= \langle\psi|\mathbb{1}\hat{X}\mathbb{1}|\psi\rangle \\ &= \int dx\, dx'\ \langle\psi|x\rangle\langle x|\hat{X}|x'\rangle\langle x'|\psi\rangle\end{aligned}$$

We know, from studying the eigenvalue problem of $\hat{X}$, that

$$\langle x|\hat{X}|x'\rangle = x\delta(x-x')$$

So, we have

$$\begin{aligned}\langle\psi|\hat{X}|\psi\rangle &= \int dx\, dx'\ \langle x|\psi\rangle^* x\delta(x-x')\langle x'|\psi\rangle \\ &= \int dx\, dx'\ \delta(x-x')\psi(x)^* x\psi(x') \\ &= \int dx\ \psi(x)^* x\psi(x)\end{aligned}$$

Therefore, the expecation value of $\hat{X}$ is

$$\boxed{\langle\psi|\hat{X}|\psi\rangle = \int dx\ \psi(x)^* x\psi(x)}$$

4. In momentum space, the momentum operator $\hat{P}$ acts on a state $\mid \psi\rangle$ as

$$\hat{P} \mid \psi\rangle \rightarrow -i\hbar\frac{d\psi(x)}{dx}$$

Or more precisely,

$$\langle x|\hat{P}|\psi\rangle = -i\hbar\frac{d\psi(x)}{dx}$$

Now, the expectation value for the momentum operator is given by

$$\begin{aligned}\langle\psi|\hat{P}|\psi\rangle &= \langle\psi|\mathbb{1}\hat{P}\mathbb{1}|\psi\rangle \\ &= \int dx\, dx'\ \langle\psi|x\rangle\langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle \\ &= \int dx\, dx'\ \langle x|\psi\rangle^*\langle x|\hat{P}|x'\rangle\langle x'|\psi\rangle\end{aligned}$$

From our earlier studies of the momentum operator, we know that the matrix elements of the operator in the position space are given by

$$\langle x|\hat{P}|x'\rangle = -i\hbar\frac{d}{dx}\psi(x)$$

So, we have

$$\begin{aligned}\langle\psi|\hat{P}|\psi\rangle &= \int dx\, dx'\ \psi(x)^* \left(-i\hbar\frac{d}{dx}\delta(x-x')\right)\psi(x') \\ &= \int dx\ \psi(x)^* \left(-i\hbar\frac{d}{dx}\right)\psi(x)\end{aligned}$$

Therefore, the expecation value of the momentum operator can be found in position space as

$$\boxed{\langle\psi|\hat{P}|\psi\rangle = \int dx\ \psi(x)^* \left(-i\hbar\frac{d}{dx}\right)\psi(x)}$$

5. The operator $\hat{P}^2$ can be thought as

$$\begin{aligned}\hat{P}^2 &= \hat{P}\cdot\hat{P} \\ &= \left(-i\hbar\frac{d}{dx}\right)\cdot\left(-i\hbar\frac{d}{dx}\right) \\ &= -\hbar^2\frac{d^2}{dx^2}\end{aligned}$$

and the matrix elements of this operator should be given by

$$\langle x|\hat{P}^2|x'\rangle = -\hbar^2\frac{d^2}{dx^2}\delta(x-x')$$

So, the expectation value of the squared momentum operator can be found as

$$\begin{aligned}\langle\psi|\hat{P}^2|\psi\rangle &= \langle\psi|\mathbb{1}\hat{P}^2\mathbb{1}|\psi\rangle \\ &= \int dx\, dx'\ \langle\psi|x\rangle\langle x|\hat{P}^2|x'\rangle\langle x'|\psi\rangle \\ &= \int dx\, dx'\ \psi(x')^*\left(-\hbar^2\frac{d^2}{dx^2}\delta(x-x')\right)\psi(x) \\ &= \int dx\ \psi(x)\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi(x)\end{aligned}$$

Therefore, the expectation value for $\hat{P}^2$ is

$$\boxed{\langle\psi|\hat{P}^2|\psi\rangle = \int dx\ \psi(x)\left(-\hbar^2\frac{d^2}{dx^2}\right)\psi(x)}$$

6. We have a system with potential $V(x)$ and hamiltonian $\hat{H} = \frac{\hat{P}^2}{2m} + V$.
<u>TISE:</u> The Time Independent Schrödinger Equation is

$$\hat{H} \mid E\rangle = E \mid E\rangle$$

In position space, the left hand side becomes

$$\begin{aligned}\langle x|\hat{H}|E\rangle &= \langle x \mid \left(\frac{\hat{P}^2}{2m} + V\right) \mid E\rangle \\ &= \langle x| \left[\left(\frac{\hat{P}^2}{2m} + V\right)|E\rangle\right] \\ &= \frac{1}{2m}\langle x|\hat{P}^2|E\rangle + \langle x|V|E\rangle\end{aligned}$$

From our earlier studies, we know that

$$\langle x|\hat{P}^2|E\rangle = -\hbar\frac{d^2}{dx^2}\psi_E(x) \quad \text{and} \quad \langle x|V|E\rangle = V(x)$$

Thus, the left hand side of the TISE is

$$\hat{H} \mid E\rangle = -\frac{\hbar}{2m}\frac{d^2}{dx^2}\psi_E(x) + V(x) \tag{5.2}$$

The expression on the right hand, $E \mid E\rangle$, in the position-space is simply

$$\langle x|E|E\rangle = E\langle x|E\rangle = E\psi_E(x) \tag{5.3}$$

So combining our results from equations (5.2) and (5.3), we find that the TISE in position-space is

$$\boxed{-\frac{\hbar}{2m}\frac{d^2}{dx^2}\psi_E(x) + V(x) = E\psi_E(x)}$$

<u>TDSE:</u> The Time-Dependent Schrödinger Equation says

$$i\hbar\frac{d}{dt} \mid \psi(t)\rangle = \hat{H} \mid \psi(t)\rangle$$

Now, the left-hand expression in position space is

$$\langle x|\left(i\hbar\frac{d}{dt}\right)|\psi(t)\rangle = i\hbar\frac{d}{dt}\langle x|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\psi_E(x,t)$$

where we are able to pull out the linear operator $\left(i\hbar\frac{d}{dt}\right)$ because it is a unitary operator, and inner products are invariant under unitary translations.

The right hand expression, expressed in position-space, is

$$\begin{aligned}
\langle x|\hat{H}|\psi(t)\rangle &= \langle x|\left(\frac{\hat{P}^2}{2m} + V\right)|\psi(t)\rangle \\
&= \frac{1}{2m}\langle x|\hat{P}^2|\psi(t)\rangle + \langle x|V|\psi(t)\rangle \\
&= \frac{-\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi_E(x,t) + V(x)\psi_E(x,t) \\
&= \left[\frac{-\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_E(x,t)
\end{aligned}$$

So, in position-space, the TDSE is expressed as

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi_E(x,t) = \left[\frac{-\hbar}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi_E(x,t)}$$

<u>Problem 3:</u>

1. We have a particle confined to the x-axis whose wavefunction is described by

$$\psi = \begin{cases} 0 & x \leq -a \\ C & -a \leq x \leq a \\ 0 & c \geq a \end{cases}$$

where C is a normalization constant.

We can find C using the normalization condition

$$\int_{-\infty}^{\infty} dx \; |\psi(x)|^2 = 1$$

We have

$$\begin{aligned} & 0 + \int_{-a}^{a} dx \; |C|^2 + 0 = 1 \\ \implies & C^2 \int_{-a}^{a} dx = 1 \quad \text{(By Convention, } C \in \mathbb{R} \text{ so } |C| = C) \\ \implies & C^2 \cdot (2a) = 1 \end{aligned}$$

Thus,

$$\boxed{C = \frac{1}{\sqrt{2a}}}$$

2. The expectation value for $\hat{X}$ is given by

$$\begin{aligned} \langle \hat{X} \rangle &= \int_{-\infty}^{\infty} \psi(x)^* x \psi(x) \\ &= 0 + \int_{-a}^{a} dx \; \left(\frac{1}{\sqrt{2a}}\right)^* x \left(\frac{1}{\sqrt{2a}}\right) + 0 \\ &= \frac{1}{2a} \int_{-a}^{a} dx \; x \\ &= \frac{1}{2a} \cdot \left[\frac{x^2}{2} \Big|_{-a}^{a} \right] \\ &= \frac{1}{2a} \cdot \left(\frac{a^2}{2} - \frac{a^2}{2} \right) \\ &= 0 \end{aligned}$$

So, the expected position is $\boxed{\langle \hat{X} \rangle = 0}$.

The expectation value for $\hat{X}^2$ is given by

$$
\begin{aligned}
\langle \hat{X} \rangle &= \int_{-\infty}^{\infty} \psi(x)^* x^2 \psi(x) \\
&= 0 + \int_{-a}^{a} dx \, \left(\frac{1}{\sqrt{2a}} \right)^* x^2 \left(\frac{1}{\sqrt{2a}} \right) + 0 \\
&= \frac{1}{2a} \int_{-a}^{a} dx \, x^2 \\
&= \frac{1}{2a} \cdot \left[\frac{x^3}{3} \bigg|_{-a}^{a} \right] \\
&= \frac{1}{2a} \cdot \left(\frac{a^3}{3} + \frac{a^3}{3} \right) \\
&= \frac{1}{2a} \cdot a^3 \\
&= \frac{a^2}{2}
\end{aligned}
$$

So, the expected position is $\boxed{\langle \hat{X}^2 \rangle = \frac{a^2}{2}}$.

3. There are some values of momentum p_x which the probability to find the particle in is zero. Our goal is to find these momenta.

Recall that the probability of having a particular momentum p is given by $|\langle p|\psi\rangle|^2$.

Inserting completeness (in the position-space), we can write

$$\begin{aligned}
\langle p|\psi\rangle &= \int dx\ \langle p|x\rangle\langle x|\psi\rangle \\
&= \int_{-\infty}^{\infty} dx\ \langle x|p\rangle^*\langle x|\psi\rangle \\
&= \int_{-\infty}^{\infty} dx\ (\psi_p(x)^*)(\psi(x)) \\
&= \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}}\right)\psi(x) \\
&= 0 + \int_{-a}^{a} dx\ \left(\frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{ipx}{\hbar}}\right)\cdot\left(\frac{1}{\sqrt{2a}}\right) + 0 \\
&= \frac{1}{\sqrt{2a}}\cdot\frac{1}{\sqrt{2\pi\hbar}}\int_{-a}^{a} e^{-\frac{ipx}{\hbar}} \\
&= \frac{1}{\sqrt{2a}}\cdot\frac{1}{\sqrt{2\pi\hbar}}\left[\frac{-\hbar}{ip} e^{-\frac{ipx}{\hbar}}\right]_{-a}^{a} \\
&= \frac{1}{\sqrt{2a}}\cdot\frac{1}{\sqrt{2\pi\hbar}}\left[\frac{i\hbar}{p} e^{-\frac{ipx}{\hbar}}\right]_{-a}^{a} \\
&= \frac{1}{\sqrt{2a}}\cdot\frac{1}{\sqrt{2\pi\hbar}}\cdot\frac{i\hbar}{p}\left[e^{-\frac{ipx}{\hbar}}\right]_{-a}^{a} \\
&= \frac{i}{2p}\cdot\sqrt{\frac{\hbar}{\pi a}}\left(e^{-\frac{ipa}{\hbar}} - e^{\frac{ipa}{\hbar}}\right) \\
&= \frac{i}{2p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot(-2)\sinh\left(\frac{ipa}{h}\right)
\end{aligned}$$

That is

$$\boxed{\langle p|\psi\rangle = \frac{-i}{p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot\sinh\left(\frac{ipa}{h}\right)}$$

Further, we can note that $\sinh(z) = -i\sin(iz)\ \ \forall z \in \mathbb{C}$ which means

$$\begin{aligned}
\frac{-i}{p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot\sinh\left(\frac{ipa}{h}\right) &= \frac{-i}{p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot(-i)\sin\left(-\frac{pa}{h}\right) \\
&= \frac{-i\cdot i}{p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot\sin\left(\frac{pa}{h}\right) \\
&= \frac{1}{p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot\sin\left(\frac{pa}{h}\right)
\end{aligned}$$

so,

$$\boxed{\langle p|\psi\rangle = \frac{1}{p}\cdot\sqrt{\frac{\hbar}{\pi a}}\cdot\sin\left(\frac{pa}{h}\right)}$$

Now, since this is a real number, we have

$$\langle\psi|p\rangle = \langle p|\psi\rangle^* = \langle p|\psi\rangle$$

Which means the probability of the particle posessing the momentum p is

$$\mathcal{P}(p) = \left[\frac{1}{p} \cdot \sqrt{\frac{\hbar}{\pi a}} \cdot \sin\left(\frac{pa}{h}\right)\right]^2$$

The momenta whose probabilities of ocurring are given by

$$\mathcal{P}(p) = 0$$

In order for this to be the case, we must have

$$\sin\left(\frac{pa}{\hbar}\right) = 0$$

So, we have

$$\begin{aligned} \frac{pa}{\hbar} &= \pi n \\ \implies p &= \frac{n\pi\hbar}{a} \end{aligned}$$

Therefore, the momenta of zero probability are given by

$$\boxed{p = \frac{n\pi\hbar}{a}, \quad n \in \mathbb{Z}}$$