What is $\hat{P}|x\rangle$?

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Abstract

Investigations into the interplay between Hilbert Space and L^2 -Space

This set of notes was inspired by Prof Valerio Scarani's Course PC2130 (QM1), and my discussions with Mr Sim Jian Xian and Prof Kuldip Singh.

1 Introduction

It seems like there is a severe lack of emphasis on the interplay between Hilbert Space, L^2-Space, and how to transition between these 2 equivalent pictures in our NUS physics education. This document is designed to alleviate this problem.

We will be working in the position basis mainly.

A quick reminder of what we already know:

$$\hat{X}|\psi\rangle = \int_{\mathbb{R}} x|x\rangle\langle x|dx \int_{\mathbb{R}} \psi(x')|x'\rangle dx' = \int_{\mathbb{R}}\int_{\mathbb{R}} x|x\rangle\langle x|x'\rangle\psi(x')dxdx'$$

$$= \int_{\mathbb{R}}\int_{\mathbb{R}} x|x\rangle\delta(x-x')\psi(x')dxdx' = \int_{\mathbb{R}} x\psi(x)|x\rangle dx$$

If we accept that commutation relations define conjugate variables, then

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

Also,

$$\hat{X}|x\rangle = x|x\rangle$$

$$\langle\hat{X}\rangle_\psi = \langle\psi|\hat{X}|\psi\rangle = \int_{\mathbb{R}} \psi^*(x)x\psi(x)dx$$

$$\langle\hat{P}\rangle_\psi = \langle\psi|\hat{P}|\psi\rangle = -i\hbar\int_{\mathbb{R}} \psi^*(x)\frac{d}{dx}\psi(x)dx$$

Except that the way some of these are presented is very misleading and not good for pedagogy! A couple of questions to motivate the point of this set of notes:

1)How did we really get from $\hat{P}|\psi\rangle$ to $\int_{\mathbb{R}} -i\hbar\frac{d}{dx}\psi(x)|x\rangle dx$?

2)What's the representation of $\hat{P}$ in L^2-Hilbert mixed representation, a la $\int_{\mathbb{R}} x|x\rangle\langle x|dx$?

3)How is the L^2 representation related to the bra-ket representation?

4)When, why, and how can we swap an L^2-derivative $i\hbar\frac{d}{dx}$ with the bra/ket?

A full presentation should talk about L^2 -Space entirely with no reference to bras and kets, then bring on bras and kets, and finally explain the transition between the two, in my opinion. Let's proceed.

2 L^2 representation

Average X =

$$\int_{-\infty}^{\infty} x \times pdf(x)dx = \int_{-\infty}^{\infty} x|\psi(x)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x)x\psi(x)dx$$

Average P =

$$\int_{-\infty}^{\infty} \psi^*(x)(-i\hbar)\frac{d\psi(x)}{dx}dx$$

(this is our starting point, I will not justify this in this article. I have seen some explanation but so far none that I am particularly happy with.)

3 Mixed representation and bra-ket representation

Now, we use $\psi(x) = \langle x|\psi\rangle$, linking the L^2 representation with the Hilbert Space representation to produce the mixed representation.
Average X =

$$\int_{-\infty}^{\infty} \psi^*(x)x\psi(x)dx = \int_{-\infty}^{\infty} (\langle x|\psi\rangle)^\dagger x\langle x|\psi\rangle dx = \int_{-\infty}^{\infty} \langle\psi|x\rangle x\langle x|\psi\rangle dx$$

$$= \langle\psi|(\int_{-\infty}^{\infty} |x\rangle x\langle x|dx)|\psi\rangle = \langle\psi|\hat{X}|\psi\rangle = \langle\hat{X}\rangle$$

We can thus identify the operator X in the mixed representation $\hat{X} = \int_{-\infty}^{\infty} |x\rangle x\langle x|dx$, and the last 2 expressions are in the bra-ket representation.

Average P =

$$\int_{-\infty}^{\infty} \psi^*(x)(-i\hbar)\frac{d\psi(x)}{dx}dx = -i\hbar\int_{-\infty}^{\infty} (\langle x|\psi\rangle)^\dagger\frac{d\langle x|\psi\rangle}{dx}dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \langle\psi|x\rangle \frac{d\langle x|\psi\rangle}{dx} dx$$

Here it should be clear that we need to pull the ket out and repeat what we did previously. However, this would obviously need to necessitate $\frac{d\langle x|\psi\rangle}{dx} = \frac{d\langle x|}{dx}|\psi\rangle$.

We are reminded that $|\psi\rangle$ itself is a state. It makes no reference to position. In fact, it's only time-dependent. This means that $\frac{d|\psi\rangle}{dx} = 0$. Thus, by the product rule, $\frac{d\langle x|\psi\rangle}{dx} = \frac{d\langle x|}{dx}|\psi\rangle$ immediately.

Continuing, Average P =

$$-i\hbar \int_{-\infty}^{\infty} \langle\psi|x\rangle \frac{d\langle x|\psi\rangle}{dx} dx = -i\hbar \int_{-\infty}^{\infty} \langle\psi|x\rangle \frac{d\langle x|}{dx}|\psi\rangle dx$$

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

We can thus identify the operator P in the mixed representation as $\hat{P} = -i\hbar \int_{-\infty}^{\infty} |x\rangle \frac{d\langle x|}{dx} dx$. [1]

Now it should be clear that $\frac{d\langle x|}{dx}$ does not mean the derivative is acting directly on $\langle x|$. To see this, we invoke the definition of a derivative $\frac{d\langle x|}{dx} = lim_{h\to 0} \frac{\langle x+h| - \langle x|}{h}$. Since $\langle x+h|$ is manifestly orthogonal to $\langle x|$ except when h=0(by the construction of the position basis), there is no convergence of the limit and thus no sensible meaning in interpreting the derivative as acting on the position basis. Instead, this should be thought of as the derivative waiting to act on the spatial wavefunction which is born of the P operator acting on a ket. In equation,

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

$$= -i\hbar \int_{-\infty}^{\infty} \frac{d\psi(x)}{dx} |x\rangle dx$$

Now we can see that $\frac{d\psi(x)}{dx}$ is essentially the new wavefunction and so at each value of x, it is essentially a constant and it can be swapped with the position basis ket. In some sense, this answers our 4th question posed at the start of the article: we can swap derivatives with bras/kets if it is clear what the derivative

[1] Some people may be uncomfortable seeing $\frac{d\langle x|}{dx}$, in which case there is a cosmetic fix by multiplying the expression with an identity

$$\hat{P}\mathbb{1} = -i\hbar \int_{-\infty}^{\infty} |x\rangle \frac{d\langle x|}{dx} dx \int_{-\infty}^{\infty} |x'\rangle\langle x'| dx' = -i\hbar \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |x\rangle \frac{d\langle x|x'\rangle}{dx} \langle x'| dx dx'$$

$$= -i\hbar \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |x\rangle \frac{d\delta(x-x')}{dx} \langle x'| dx dx' = -i\hbar \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |x\rangle \delta'(x-x') \langle x'| dx dx'$$

which look slightly less intimidating but is honestly not much better when you think of how to deal with $\delta'(x-x')$.

is acting on(the wavefunction, when it appears). So in some sense, we can write $\hat{P}|\psi\rangle = -i\hbar \int_{-\infty}^{\infty} \frac{d|x\rangle}{dx}\langle x|dx$ since it is clear what the derivative should be acting on, although we can all agree that that would be much more misleading. It is thus perhaps more illuminating to write $\hat{P} = -i\hbar \int_{-\infty}^{\infty} |x\rangle \frac{d}{dx}\langle x|dx$, so it is clear that the position basis kets are waiting for a $|\psi\rangle$ to project on it, and the derivative is waiting to act on the projection which gives the wavefunction. With this, we can answer the question in the title of the article.

$$\hat{P}|x_0\rangle = -i\hbar \int_{-\infty}^{\infty} |x\rangle \frac{d}{dx}\langle x|x_0\rangle dx = -i\hbar \int_{-\infty}^{\infty} |x\rangle \frac{d}{dx}\delta(x-x_0)dx$$

$$= -i\hbar \int_{-\infty}^{\infty} |x\rangle \delta^{'}(x-x_0)dx = -i\hbar \int_{-\infty}^{\infty} \delta^{'}(x-x_0)|x\rangle dx$$

The fact that this expression is not very well-defined(since $\delta^{'}(x-x_0)$ is waiting to act on something[2]) corresponds to the fact that it is not very physically meaningful to have the momentum operator act on a position basis.

It is tempting but wrong to try to evaluate this directly as follows

$$-i\hbar \int_{-\infty}^{\infty} \delta^{'}(x-x_0)|x\rangle dx = -i\hbar \int_{-\infty}^{\infty} \delta^{'}(x-x_0)(1)|x\rangle dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \delta(x-x_0)\frac{d(1)}{dx}|x\rangle dx = -i\hbar \int_{-\infty}^{\infty} \delta(x-x_0)(0)|x\rangle dx = 0$$

It is important to remember that fundamentally this is still an operator[3] and it is waiting to act on something. For an example of what it acts on, refer to the next section for the hermitian conjugated case.

4 Addendum on $\hat{P}$

In some stackexchange posts you may see this expression

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

or

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

Given our explicit expression of $\hat{P}$ in the mixed representation, it is now clear why that is true.

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

[2]refer to the wiki if need be https://en.wikipedia.org/wiki/Dirac_delta_function#Derivatives_of_the_Dirac_delta_function

[3]The technical reason is that as a distribution, it is only defined on compactly supported smooth test functions. 1 is not compactly supported, so the $\delta^{'}$ would not be acting on it, and thus it is still waiting for something to act on

$$= -i\hbar \int_{-\infty}^{\infty} \frac{d\psi(x')}{dx'} \delta(x - x') dx' = -i\hbar \frac{d\psi(x)}{dx} \int_{-\infty}^{\infty} \delta(x - x') dx'$$

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

Similarly,

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

$$= -i\hbar \int_{-\infty}^{\infty} \delta(x - x') \frac{d}{dx'} \langle x'|dx' = -i\hbar \frac{d}{dx} \langle x| \int_{-\infty}^{\infty} \delta(x - x') dx' = -i\hbar \frac{d}{dx} \langle x|$$

Recall that previous we have a $\delta^{'}(x - x')$ when we act $\hat{P}$ on $|x\rangle$. Given that $\langle x|\hat{P}$ is the hermitian conjugates of $\hat{P}|x\rangle$, verify that $\langle x|\hat{P}|\psi\rangle$ is consistent with the hermitian conjugate of $\langle\psi|\hat{P}|x\rangle$ by referring to the wiki for $\delta^{'}(x - x')$.

5 References

Prof Valerio's final rendition of PC2130 notes

Prof Ho Wen Wei's first set of PC2130 notes

Prof Kuldip's NST2014 Formalism notes

https://physics.stackexchange.com/questions/113808/what-is-hatpx-rangle?noredirect=1&lq=1

https://physics.stackexchange.com/questions/76299/how-does-the-momentum-operator-act-on-state-kets