1 Operators in quantum mechanics

(In case Quantum Fundamentals hasn't covered this yet.) An **operator** in quantum mechanics corresponds to a linear transformation of a state (or ket). In a matrix representation, an operator would be a matrix, and would transform a column vector to another column vector by matrix multiplication. We represent operators with hats, such as $\hat{S}_z$.

Any quantity that we could observe, like the spin or position of a particle has a corresponding Hermitian operator. The eigenvalues of the operator corresponding to an obsevables are the set of values that could be measured when that observable is measured. For instance, the z component of the spin $\hat{S}_z$ for a spin-$\frac{1}{2}$ particle has eigenvalues of $\pm\frac{1}{2}\hbar$, which is why only those two spin values are measured.

Any operator can be written as a matrix using any basis set (of the corresponding system). The elements of that matrix, which represents the operator, are called **matrix elements**, and are given by $O_{ij} \equiv \langle i|\,\hat{O}\,|j\rangle$, where $|i\rangle$ and $|j\rangle$ are two basis states, $\hat{O}$ is some operator, and O_{ij} is an elment of the matrix corresponding to that operator.

2 Operators on wave functions

A **wave function** represents the **state** of a particle in space, just as a ket or an array of two elements represents the state of a spin-$\frac{1}{2}$ particle. Just as there are operators for spins that relate to physical observables, there are also operators for particles in space, which act on wave functions.

We will be considering just one operator this week: the position operator. The position operator in the wave function representation is given by

$$\hat{x} \doteq x \tag{1}$$

You might have some trouble understanding what this means, given that the hat and the dot are both new notations. I'll try to explain element by element.

$\hat{x}$ This is the operator corresponding to the classical observable x. When we write an operator with a hat like this, we are being abstract in terms of what representation we are using. **Warning! We annoyingly use the same notation for a unit vector in the x direction in Cartesian coordinates! This is unfortunate, but context should allow you to identify the meaning of the hat.**

$\doteq$ This means that the thing on the left (which is representation-independent) can be represented (often in a particular basis) by the thing on the right (which is specific to that representation/basis).

x This is the representation of the position operator in the wave function representation, which we can also call the position basis, since it is the representation in which $\hat{x}$ is represented by x. In contrast, next quarter you will learn about a momentum basis, in which $\hat{x} \doteq i\hbar\frac{\partial}{\partial p}$.

Last week we explored how we can represent a wave function in a sinusoidal basis. Today we will explore how to represent the position operator in the sinusoidal basis. In order to do this, we will compute what

is called a **matrix element**. The matrix element is defined by

$$x_{nm} = \langle n|\hat{x}|m\rangle \tag{2}$$

$$= \int \phi_n^*(x) x \phi_m(x) dx \tag{3}$$

and you can think it as one of the "elements" that shows up in a matrix.

2.1 Why is this thing a "matrix element"?

Recall that we started by finding the average position, which was

$$\langle x\rangle = \int \mathcal{P}(x) x dx \tag{4}$$

$$= \int |\psi(x)|^2 x dx \tag{5}$$

$$= \langle\psi|\hat{x}|\psi\rangle \tag{6}$$

You then found that you could write $\psi(x)$ as a sum of basis functions

$$|\psi\rangle = \sum_{n=1}^{\infty} C_n |n\rangle \tag{7}$$

$$= \sum_{n=1}^{\infty} \langle n|\psi\rangle |n\rangle \tag{8}$$

and thus

$$\psi(x) = \sum_{n=1}^{\infty} C_n \phi_n(x) \tag{9}$$

We can now put these two expressions together by substituting the expressions for $\psi(x)$ into the expression for $\langle x\rangle$:

$$\langle x\rangle = \int \psi(x)^* x \psi(x) dx \tag{10}$$

$$= \int \left(\sum_{n=1}^{\infty} C_n \phi_n(x)\right)^* x \left(\sum_{n=1}^{\infty} C_n \phi_n(x)\right) dx \tag{11}$$

At this point we run into a possible confusion. I've written down two summations with the same summation index. This is a natural outcom of plugging in the equation for $\psi(x)$, but we've now got two different index variables with the same name. Whenever this happens to you, it's a good idea to change the equation to give them different names. Since we're summing over them, these index variables are "dummy indexes", just as our integral variable x is a "dummy variable" and could be renamed at will. We could change one of them to n' or we could change one of them to m. I'll pick the latter.

$$\langle x\rangle = \int \left(\sum_{n=1}^{\infty} C_n \phi_n(x)\right)^* x \left(\sum_{m=1}^{\infty} C_m \phi_m(x)\right) dx \tag{12}$$

Now that we have different dummy variables for summation, we can pull reorder our summations and pull them out of the integral

$$\langle x \rangle = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} C_n^* C_m \int \phi_n(x)^* x \phi_m(x) dx \tag{13}$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} C_n^* C_m \langle n|\hat{x}|m\rangle \tag{14}$$

$$= \begin{pmatrix} C_1^* & C_2^* & C_2^* & \cdots \end{pmatrix} \begin{pmatrix} \langle 1|\hat{x}|1\rangle & \langle 1|\hat{x}|2\rangle & \langle 1|\hat{x}|3\rangle & \cdots \\ \langle 2|\hat{x}|1\rangle & \langle 2|\hat{x}|2\rangle & \langle 2|\hat{x}|3\rangle & \cdots \\ \langle 3|\hat{x}|1\rangle & \langle 3|\hat{x}|2\rangle & \langle 3|\hat{x}|3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_2 \\ \vdots \end{pmatrix} \tag{15}$$

$$= \langle \psi|\hat{x}|\psi\rangle \tag{16}$$

Thus we can see that the $\hat{x}$ operator does seem to be represented in our sinusoidal basis as a matrix of infinite dimension with its elements given by $x_{nm} = \langle n|\hat{x}|m\rangle$. Thus we can also write that

$$\hat{x} \doteq \begin{pmatrix} \langle 1|\hat{x}|1\rangle & \langle 1|\hat{x}|2\rangle & \langle 1|\hat{x}|3\rangle & \cdots \\ \langle 2|\hat{x}|1\rangle & \langle 2|\hat{x}|2\rangle & \langle 2|\hat{x}|3\rangle & \cdots \\ \langle 3|\hat{x}|1\rangle & \langle 3|\hat{x}|2\rangle & \langle 3|\hat{x}|3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{17}$$

meaning that in the *sinusoidal* basis the x position operator is represented by this matrix.

3 Your task

1. Write a function that given n and m solves for and returns $\langle n|\hat{x}|m\rangle$. Please do your integrals numerically. *(Yes, these integrals can be done analytically, but that is a bit of a pain, and this is a computational course.)*

2. Create a matrix (or 2D array) for the position operator $\hat{x}$. You'll have to choose a maximum value of n to make this a finite matrix. Please pick something practical, but reasonably big. **This is going to require that you index your array. In python, as with most programming languages, arrays are indexed starting with zero, so the index you will put into the array will be one less than the value of n that you mean.**

3. Visualize this matrix with a color plot. **Raise your hand when you have visualized the position operator matrix!** Try increasing the number of basis functions included. *Does the matrix seem to "converge" like your wavefunctions did last week?*

4 Your next task

Once you have a matrix (or 2D array) corresponding to the position operator in the sinusoidal basis, we will want to determine the eigenstates and eigenvalues of the position operator. Those eigenstates

can be expressed in more than one representation. Because the position matrix you construct is in the representation of our sinusoidal basis set, the eigenvectors that you obtain will also be in that representation.

$$\hat{x}|v_i\rangle = \lambda_i|v_i\rangle \tag{18}$$

$$\begin{pmatrix} \langle 1|\hat{x}|1\rangle & \langle 1|\hat{x}|2\rangle & \langle 1|\hat{x}|3\rangle & \cdots \\ \langle 2|\hat{x}|1\rangle & \langle 2|\hat{x}|2\rangle & \langle 2|\hat{x}|3\rangle & \cdots \\ \langle 3|\hat{x}|1\rangle & \langle 3|\hat{x}|2\rangle & \langle 3|\hat{x}|3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} v_{i1} \\ v_{i2} \\ v_{i3} \\ \vdots \end{pmatrix} = \lambda_i \begin{pmatrix} v_{i1} \\ v_{i2} \\ v_{i3} \\ \vdots \end{pmatrix} \tag{19}$$

$$|v_i\rangle = \sum_{n=1}^{\infty} v_{in}|n\rangle \tag{20}$$

$$v_i(x) = \sum_{n=1}^{\infty} v_{in}\phi_n(x) \tag{21}$$

1. Solve for the eigenvalues and eigenvectors of the position matrix (`numpy` has a function to do this).
2. Visualize a few of the eigenfunctions of the position operator. These eigenfunctions are given by

$$v_i(x) = \sum_{n=1}^{\infty} v_{in}\phi_n(x) \tag{22}$$

3. On the same graph (with the eigenfunctions) visualize the corresponding eigenvalues as vertical lines. **Raise your hand when you have visualized at least a couple of eigenfunctions of the position operator along with their corresponding eigenvalues!**
4. Try increasing the size of your matrix, and see how the eigenvalues and eigenfunctions change. *What do the eigenfunctions seem to be converging to?*

Paper fun Solve analytically for the eigenstates of the position operator *in a wave function representation.* Compare them with your approximate numerical eigenstates above.

To do this, you'll want to try picking a function, any function, and then sketch that function and x times that function. If they look the same, you found the eigenfunction. Otherwise try again.

> **Solution** *Note that to solve this in a reasonable way (if you don't already know the answer) it is really important to be able to in a sketch multiply two functions. This is an invaluable skill, and well worth practicing!*
>
> To do this, we can begin with any guess we want. The simplest is probably an $n = 1$ sinusoid. We sketch $\sqrt{\frac{2}{L}}\sin(\pi x/L)$, which has one symmetrical bump. If we multiply by x, we find that the right-hand side gets bigger relative to the left-hand side. It's not the same shape.
>
> We can then pick another function, like you might try a function that is zero on the left-hand side of the box, and is a sinusoid on the right-hand side:
>
> $$f(x) = \begin{cases} 0 & x < L/2 \\ -\sin(2\pi x/L) & x \geq L/2 \end{cases} \tag{23}$$

This just looks like the previous function, but squished and scooted to the right. And I didn't bother normalizing it. If we multiply this function by x, again the right-hand side of the peak is increased relative to the left-hand side, but now the distortion is not as big. Because we made the peak skinnier, x had a smaller fractional change from one side to the other.

Moral of the story: a skinnier function (with zero elsewhere) will be closer to an eigenfunction of $\hat{x}$. We can continue this process, making the function skinnier and skinnier, until we have a function that is non-zero at only one point in space. And the x value of that point in space will be the eigenvalue. This gets us to the Dirac δ function, which is the eigenfunction of the position operator. It's not a well-behaved function, which is why I didn't start with this.

Meaning of results You constructed a matrix that represents the $\hat{x}$ operator in the sinusoidal basis set. Doing this required computing matrix elements, which are kind of like inner products, but have an operator sandwiched in the middle. `numpy` then solved for the eigenvalues and eigenvectors of this matrix, which gave you an approximation for the eigen*functions* of the position operator. These were only approximations, because we did not include all of the infinite number of sinusoidal basis functions. When you looked at the eigenvalues, you may have noticed that they are equally spaced from 0 to L. The eigenfunctions of $\hat{x}$ are functions that have a single well-defined position, which well-describes the Dirac δ function.

We can show that $\delta(x - x_0)$ is an eigenfunction of x because

$$x\delta(x - x_0) = x_0\delta(x - x_0) \qquad \text{for all } x \tag{24}$$

thus $\delta(x - x_0)$ is an eigenfunction of $\hat{x}$ with eigenvalue x_0.

Extra-advanced subtlety (not needed, skipped in lecture!) You might wonder about normalization. It would be natural to expect the eigenfunction to be normalized, which would lead to an expression like

$$xv_i(x) = x_i v_i(x) \tag{25}$$

$$1 = \langle v_i | v_i \rangle \tag{26}$$

$$= \int_0^L v_i(x)^* v_i(x) dx \tag{27}$$

This would lead us to conclude that $v_i(x) = \sqrt{\delta(x - x_i)}$. This is incorrect, however, although it is a mistake that faculty also make sometimes. The problem with this statement is that we actually need to normalize the eigenfunctions differently when working with a continuous basis like this.

The problem with the above is that we cannot write a discrete sum over all the basis functions in this case, as we were able to do before. Instead we are forced to use an *integral* over all the basis function, and that changese the dimensions that are needed.

In a discrete basis set, we write

$$|\psi\rangle = \sum_n C_n |n\rangle \tag{28}$$

and we "multiply" (with an inner product) each side by $\langle n'|$ on the left to find

$$\langle n'|\psi\rangle = \sum_n C_n \langle n'|n\rangle \tag{29}$$

Then we can use the orthonormality of the basis to write the right-hand inner product as a Kroenecker delta and kill the sum:

$$\langle n'|\psi\rangle = \sum_n C_n \delta_{nn'} \tag{30}$$

$$\langle n'|\psi\rangle = C_{n'} \tag{31}$$

Why did I do all this? To give an example of how we use basis functions, since one use for eigenfunction is often to form a useful basis set.

When doing the same process with $\hat{x}$ eignefunctions, we run into some trouble: because x varies continuously, we cannot write a sum over all possible x. Between any two x (that are not equal to one another) there are an infinite number of other x values. So instead of a sum, we are forced to use an integral:

$$|\psi\rangle = \int C_x |x\rangle \, dx \tag{32}$$

where I am taking $|x\rangle$ to mean the eigenfunction that has eigenvalue x, and C_x to be the corresponding coefficient. We can proceed as we did in (29):

$$\langle x'|\psi\rangle = \langle x'| \int C_x |x\rangle \, dx \tag{33}$$

$$= \int C_x \langle x'|x\rangle \, dx \tag{34}$$

At this point we need to think about what $\langle x'|x\rangle$ is. In (30) we treated an inner product like this as a Kronecker delta (which indicated orthonormality), but a Kronecker delta requires that the two indices be integers. The corresponding quantity here is a Dirac δ function, i.e. $\langle x'|x\rangle = \delta(x - x')$, which would result in

$$\langle x'|\psi\rangle = \int C_x \delta(x - x') dx \tag{35}$$

$$= C_{x'} \tag{36}$$

That looks promising (and a little familiar), but it also means that our $|x\rangle$ must not be normalized. If we had chosen to normalize our $|x\rangle$ we would have run into trouble. This $\langle x'|x\rangle = \delta(x - x')$ also relates to the dimensions of $|x\rangle$, since the delta function has dimensions of inverse distance means that $|x\rangle$ must have different dimensions from $|\psi\rangle$, which is distinctly weird.

Completeness relation

$$1 = \int |x\rangle \langle x| \, dx \tag{37}$$