H Operators

1. Before we proceed further there is a new quantity we need to define. This quantity is called an operator. An operator is a quantity that "operates" on any element of a vector space and yields another element of the vector space:

$$\mathcal{O} \left| \eta \right\rangle = \left| \chi \right\rangle \tag{H.6}$$

   Where $\left| \eta \right\rangle$ and $\left| \chi \right\rangle$ are *ket* vectors belonging to some n-dimensional vector space.

2. For simplicity we could look at rotation operators in 3-dimensions. For example, consider the unit vector $\hat{\imath}$ in 3-dimensions. A rotation operator about the z-axis converts $\hat{\imath} \rightarrow \hat{\jmath}$, the unit vector along the y-direction. Such a rotation operator conforms to the definition in Eq. (H.6) and is hence an operator in this sense. But this definition also applies to any general transformation in three-dimensions that takes an arbitrary vector $\vec{r}$ to $\vec{r'}$.

3. We will see that there will be other kinds of operators we will have in quantum mechanics and later in the course there is a whole theory of operators that we will develop. Operators and vectors spaces (which we have already discussed using the Dirac notation) form a basic tool in quantum mechanics.

4. We will now introduce a specific kind of an operator. This operator is called the momentum operator and has the following form:

$$\hat{p} = -\imath\hbar \frac{\partial}{\partial x} \tag{H.7}$$

   Note that we have seen $\hbar$ before in Eq. (2.5) and the section of wave-particle duality. The full theoretical reason for the choice of the momentum operator in Eq. (H.7) is based on the analogy to generator functions for infinitesimal translation in classical mechanics. This discussion is beyond the scope of the current course, but the interested reader is encouraged to look at Section 1.6 (on page 44) of Sakurai.

5. We will see that every observable quantity has an operator associated with it in quantum mechanics and momentum is an observable quantity.

6. We noted above that an operator is one that acts on a vector and converts it to a different vector. Is it possible that an operator can act on some vector and not change it? That is,

$$\mathcal{O} \left| \eta \right\rangle = \wr \left| \eta \right\rangle \tag{H.8}$$

   where $\wr$ is a number. Is this possible? Indeed, as we will see, for every operator that we will see in this course, there will always exist "special" *ket* vectors that do not change (only get re-scaled) on the action of some operator. These "special" *ket* vectors are called *eigen-vectors* of the operator $\mathcal{O}$. Every operator has a set of *eigen-vectors*. (Yes, a set of them.) The "special" numbers $\wr$ are called the *eigenvalues*. The term *eigen* comes from German; it means *characteristic*. So we are trying to say that the set of *eigen-vectors* and *eigenvalues* are characteristic of the operator they are obtained from. We will see more on this later as we solve quantum problems.

7. Since every operator has an eigenvector, what is the eigenvector for the momentum operator in Eq. (H.7)? To answer this question, lets try the action of the momentum operator in $\exp\{\imath kx\}$:
$$-\imath\hbar\frac{\partial}{\partial x}\exp\{\imath kx\} = \hbar k\exp\{\imath kx\} \tag{H.9}$$
You can check that this is true by differentiating the left hand-side once with respect to x. It is left as **homework** for the student to prove Eq. (H.9). The eigenstates of the momentum operator may also be represented by the *ket* $|k\rangle$. (Note: $k = \frac{2\pi}{\lambda}$.)

I Theory of Operators: I

1. We may recall what operators are from our earlier discussion:

$$\mathcal{O}\left|\eta\right\rangle = \left|\chi\right\rangle \tag{I.1}$$

2. Every observable quantity has an operator associated with it

3. Eigenvalues and Eigenvectors:

$$\mathcal{O}\left|\eta\right\rangle = \wr\left|\eta\right\rangle \tag{I.2}$$

   There are special vectors of this kind associated with every operator.

4. **Linear Operators:** Consider two operators $\hat{A}$ and $\hat{B}$. These operators are considered "linear operators" if:

   (a)
$$\left[\hat{A}+\hat{B}\right]\left|\eta\right\rangle = \hat{A}\left|\eta\right\rangle + \hat{B}\left|\eta\right\rangle \tag{I.3}$$

   (b) If c is a number (may be complex) then

$$\hat{A}\left[c\left|\eta\right\rangle\right] = c\left\{\hat{A}\left[\left|\eta\right\rangle\right]\right\} \tag{I.4}$$

   (c)
$$\hat{A}\left[\left|\eta\right\rangle + \left|\chi\right\rangle\right] = \hat{A}\left|\eta\right\rangle + \hat{A}\left|\chi\right\rangle \tag{I.5}$$

5. Note: The Hamiltonian operator is a linear operator. Why? Because the derivative operator is a linear operator.

6. The product of two operators $\hat{A}$ and $\hat{B}$ is defined as follows:

$$\hat{A}\hat{B}\left|\eta\right\rangle = \hat{A}\left[\hat{B}\left|\eta\right\rangle\right] = \hat{A}\left[\left|\chi\right\rangle\right] = \left|\alpha\right\rangle \tag{I.6}$$

   where we have assumed $\hat{B}\left|\eta\right\rangle \equiv \left|\chi\right\rangle$. Note this also defines the square of an operator:

$$\hat{A}^2\left|\eta\right\rangle = \hat{A}\left[\hat{A}\left|\eta\right\rangle\right] \tag{I.7}$$

7. **Commutators:** The commutator of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{I.8}$$

8. Note that an operator $\hat{A}$ *commutes* with itself since

$$\left[\hat{A},\hat{A}\right] = \hat{A}\hat{A} - \hat{A}\hat{A} = 0 \tag{I.9}$$

9. **Anti-Commutators:** The anti-commutator of two operators $\hat{A}$ and $\hat{B}$ is defined as

$$\left[\hat{A}, \hat{B}\right]_+ = \hat{A}\hat{B} + \hat{B}\hat{A} \tag{I.10}$$

Note the "+"

10. **Homework:** Work out the following commutators:

    (a) $\left[\frac{d}{dx}, \frac{d}{dx}\right]$ = ?

    (b) $\left[x, \frac{d}{dx}\right]$= ?

    (c) $\left[f(x), \frac{d}{dx}\right]$ = ?

    (d) $\left[f(x), \frac{d}{dx}\right]_+$ = ?

    (e) $\left[\frac{d}{dx}, \frac{d}{dx}\right]_+$ = ?

    (f) $\left[\frac{d}{dx} + f(x)\right]^2$ = ?

11. **Eigenvalues and Eigenvectors**

$$\hat{A} \left|\eta\right\rangle = a \left|\eta\right\rangle \tag{I.11}$$

where a is a number, called the eigenvalue. $\left|\eta\right\rangle$ is the eigenvector.

12. **Representing operators**

    (a) Earlier we spoke about how we could "represent" vectors. That is, any vector can be represented as a linear combination of a complete set of vectors. (If this statement is not clear, please revise the linear algebra notes.)

    (b) Operators can be represented in a similar for. In fact if you have a complete set of vectors $\{\left|i\right\rangle\}$, we can write an operator as a matrix. What we mean by this is we could represent an operator using a collection of matrix elements that have the following form:

$$A_{j,l} \equiv \left\langle j \left| \hat{A} \right| l \right\rangle \tag{I.12}$$

    $A_{j,l}$ is the (j, l)-th element of the matrix that is used to represent the operator $\hat{A}$. (Make sure to compare this with the Pauli spin matrix homework so you understand whats going on clearly.)

    (c) Does this definition make sense? $\hat{A} \left|l\right\rangle$ is another vector. You could call it $\left|m\right\rangle$ if you like. In that case the right hand side of Eq. (I.12) is the "dot" product of two vectors: $\left\langle j\right|$ and $\left|m\right\rangle$. The "dot" product of two vectors is a number. Hence the definition in Eq. (I.12) makes sense. (If these arguments are not a 100% clear to you, you need to go back and revise handout on linear algebra and also the one dealing with representation theory.)

    (d) For Eq. (I.12) to be useful we should know what $\hat{A}$ does to $\left|l\right\rangle$ when it acts on it.

