**Mathematical Foundations**

**General Properties of diagonalizable operators**

Now we want to discuss what kind of operators can have eigenvectors. Not all operators have eigenvectors/eigenvalues. For instance, consider the operator, written in some basis,



Let’s try to find the eigenvectors and eigenvalues of the operator. This would necessitate solving the equation,



which requires,



Plugging the first possibility back into the matrix equation,



But this matrix equation has no non-zero solution, as you can tell by taking the inverse matrix of both sides, or graphing the resulting linear equations, or whatever. The same will be true of the other ‘eigenvalue’. If you compare this matrix to the - matrix studied before, which did have eigenvectors, you can glean some insight into why this matrix fails to have an eigenvector. It is because the ‘2’ in the lower left corner of the present matrix is not a ‘1’, like it was before. So we may extrapolate that a matrix must be symmetric about its diagonal, i.e. be equal to its transpose, to have eigenvectors. This is just about true. More generally, if a matrix is equal to the complex conjugate of its transpose, then it will have eigenvectors/eigenvalues. We call such matrices Hermitian. So a sufficient condition is that the **O** = **O**†, or more generally, that Ô = Ô†.



where N is the dimensionality of the space. We can prove some other facts about such operators that will be useful for quantum mechanics:

***1. Hermitian matrices must have real eigenvalues***

For instance let |ψa> be an eigenstate of a Hermitian operator . Then to prove that the eigenvalues of  must be real we can write,



So the eigenvalues are real. This is in congruence with the fact that all of the eigenvalues found above were in fact real.

***2. Eigenvectors with different eigenvalues are orthogonal***

We can prove that eigenvectors with different eigenvalues are orthogonal as well. Let |ψa′> be another eigenvector of  with a different eigenvalue a′. Then consider that:



If both statements are true while a and a′ are different, then it must be the case that <ψa|ψa′> = 0, and so the vectors are orthogonal. You may verify for example that for each of the operators in the previous examples, the eigenvectors corresponding to different eigenvalues were orthogonal. However, for operator M, one of its eigenvalues of degenerate. And so the two eigenvectors corresponding to that eigenvalue were not initially orthogonal – in agreement with the theorem above – though we did make them so using the projection operator. We can always make the eigenvectors orthogonal (and also orthonormal) to each other but they won’t necessarily *automatically* come out that way if their eigenvalues aren’t distinct.

**Properties of simultaneously commuting or anti-commuting operators**

The commutator of two operators is defined as follows,



and the anti-commutator of two operators is defined as:



If the commutator or anti-commutator of two Hermitian operators is zero, then some special things happen. First consider this. Let |ψa> be an eigenstate of  with eigenvalue a. And suppose  commutes with , i.e. . Then,



And so |ψa> is also an eigenstate of  with the same eigenvalue. So  maps |ψa> to another eigenvector in the (possibly) degenerate subspace of eigenvalue a. On the other hand, if , then |ψa> will lie in the (possibly) degenerate subspace of  with oppositely signed eigenvalues.



So,



Moreover, if  and  commute, then they must be simultaneously diagonalizable, meaning that we can find a set of N linearly independent vectors which are simultaneously eigenvectors for both  and . First consider the case that Â is non-degenerate. Then let |ψm> denotes a set of eigenstates of , with eigenvalues an. Then,



So then if all the *a*’s are different, and m ≠ n, then we must have that:



which means that the |ψm>’s diagonalizeas well.



So we can assert the following:



On the other hand, if some of the *a*’s are degenerate, like for instance if a3 = a4 as shown below:



then this basis will leave  block diagonal, like this:



Observe that this form is consistent with the equation:



since for the m’s, n’s such that am ≠ an, then we must have that Bmn = 0. But for the indices (i.e. 3 and 4) where the am = an, then  can be anything. Nonetheless, it would then be possible to simultaneously diagonalize the two matrices by choosing a linear combination of the ψ3 and ψ4 wavefunctions which diagonalizes in that subspace. Of course, this linear combination will still diagonalize  in that subspace. So the important thing to take away is that:



Similarly, if ,, and all commute with each other, then we can find a set of N linearly independent eigenvectors which simultaneously diagonalizes all three.

**Example: Diagonalization of operators T and O from above**

Consider the operators  and Ô above.



And consider first the eigenvectors, eigenvalues of .



And those of Ô,



 and Ô commute, as can be verified using their matrix representation:



Therefore they can be simultaneously diagonalized. Since the eigenvectors of  are non-degenerate, according to the theorem above, these should also be eigenvectors of Ô. We can explicitly verify this is the case since:



Now let’s reason in reverse. Are the eigenvectors of Ô necessarily eigenvectors of . Well, since the eigenvectors of Ô are degenerate, this isn’t necessarily the case. Indeed, if we explicitly check, we find:



So they are not. But is there a set of basis vectors which is simultaneously eigenvectors of Ô and ? Since the operators commute there must be, according to the theorem above. And there is such a basis. We already found it – it is just the eigenbasis of  in this case.



Since  is non-degenerate, this had to be the case. But if both  and Ô were both degenerate, then the simultaneous basis wouldn’t necessarily have been either of the original eigenbasis of  or Ô.

**Some more interesting stuff**

Suppose we have two Hermitian operators: A, B. Then {A,B} is Hermitian, and expectations are real.



Conversely, [A,B] is anti-Hermitian and its expectations are therefore imaginary,



**Commutation Relations**

Commutation relations show up a bit in quantum mechanics, and so it is useful to have a bunch of identities handy. Let’s use a little notation. Denote:

 as 

We can show that the commutator is a linear function.



or in other words,



Also, interestingly, the commutator works something like a derivative. Consider that:



Works the other way too,



or in other words,



which looks exactly like a product rule. Harping on the commutator as derivative thing a bit more, consider the possibility that:



where k is some constant. Then,



and,



And,



We can see this following the pattern of a derivative. We could use induction to prove that generally:



Now consider the commutator of C with a function of A. This would be:



So we can say,



We’ll use this relationship later on in the semester. A corollary is that any operator commutes with a function of itself, i.e., [A,f(A)] = 0, since AA = [A,A] = 0. And another is that if [A,B] = 0, then [A, f(B)] = 0, and [f(A),B] = 0, and even [f(A),g(B)] = 0. So in general,



Another interesting relation, easily proved this time is:



Here’s another random thing. Any operator commutes with itself obviously. This is true even when the operator is a sum of non-mutually commuting operators. Say,



and that i doesn’t commute with j, unless i = j of course. Then,



This doesn’t mean that vector operators commute with each other, though. For instance, say:



Then the outer product commutator would be:



But what we have here is a tensor operator, and we cannot just switch indices ji to ij.

**Functions of an operator**

Let be an operator. Often in the literature one will see expressions like exp(i), etc. And in the last example we of course talked about a function an operator. Let’s see how we can make sense of such expressions considering that is an operator. Let’s suppose that is Hermitian (the only kind we’ll be dealing with in quantum mechanics anyway). Then f(Â) is formally defined through the Taylor series expansion of f(x).



Now suppose the operator can be written in such a way that it is diagonal in its basis.



Then what does f(Â) look like? It looks like this:



To prove this statement let’s consider the following. We’ll calculate Âp and see what that looks like.



Now the last delta function will make p = p-1, and the next (not shown) will make p-1 = p-2, and the next (not shown) will make p-2 = p-3, and so on, until the first two make n3 = n2, and then finally n2 = n1. So the delta functions will ultimately make everything n1. So then we have:



Now finally, we want to consider an arbitrary function of  then we’ll get:



So our statement is proved. But what if our operator Â isn’t diagonal in its present basis? Then we switch to its eigenbasis in which it is diagonal So then we can say:



We can use these results to prove a nice operator identity – but we won’t. Let  and  be operators which both commute with their commutator . Then:

