Lecture 3:
Operators

In the last lecture we have associated a linear operator f to a dynamical variable. We will now proceed to study the properties of these operators and how to extract expectation values and probabilities for a measurement.

The mean value of an operator is, by definition,:

$$\langle f \rangle_\psi = \int \psi^* f \psi \, \mathrm{d}\, r \equiv \langle \psi | f | \psi \rangle, \tag{1}$$

It must be noted here that not every linear operator can represent a variable of the system. A necessary condition is that the eigenvalues of the operator must all be real. A practical definition of a real number is that of a complex number that is equal to its complex conjugate. It thus follows that:

$$\langle f \rangle_\psi = \int \psi^* f \psi \, \mathrm{d}\, r = \int (\psi^* f \psi \, \mathrm{d}\, r)^* = \langle f \rangle_\psi^* \tag{2}$$

We define here the *transpose operator* f^T as:

$$\int \phi f^T \psi \, \mathrm{d}\, r \equiv \int f \phi \psi \, \mathrm{d}\, r \qquad \forall \phi, \psi, \tag{3}$$

and also the *Hermitian conjugate* $f^\dagger$ of an operator as:

$$f^\dagger = \left(f^T\right)^* = \left(f^*\right)^T. \tag{4}$$

An operator is defined as Hermitian if $f^\dagger = f$.

3.a Example

Let us demonstrate that the following matrices are hermitian:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{5}$$

whereas the product $\sigma_1 \sigma_2$ is not. We recall that an operator is hermitian if it is equal to its Hermitian conjugate or, equivalently, to the complex conjugate of its transposed operator. We will start with σ_1. Transposing a matrix means that it must be reflected along its main diagonal, leaving σ_1 unchanged. We then need to take the complex conjugate but, since the operator is real, this is equal to the matrix itself. We thus trivially have $\sigma_1^\dagger = \sigma_1$. For σ_2 the procedure is similar, and we leave the demonstration to the reader. The product $\sigma_1\sigma_2$ reads instead:

$$\sigma_1\sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = \sigma_3 \tag{6}$$

The transpose of this matrix is the matrix itself ($\sigma_3^T = \sigma$), when we then take the complex conjugate we have:

$$\sigma_3^\dagger = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -\sigma_3 \neq \sigma_3 \tag{7}$$

■

We can now show that any Hermitian operator has real eigenvalues. We start from Eq. ??:

$$\left(\int \psi^* f \psi \, \mathrm{d}\, r\right)^* = \int (\psi^* f \psi \, \mathrm{d}\, r)^* = \int (f\psi)^* \, \psi \, \mathrm{d}\, r = \int (f^* \psi^*) \, \psi \, \mathrm{d}\, r = \int \psi^* f^\dagger \psi \, \mathrm{d}\, r \tag{8}$$

But $f^\dagger = f$, so the last member of the equation is identical to Eq. ??. An Hermitian does then have only real eigenvalues.

3.b Example

An important thing to note is that any eigenvalue of an operator must be real, but the operator itself can be complex. For instance, the operator momentum is defined as: $\vec{p} = -i\hbar\nabla$. In one dimension it reads: $p_x = -i\hbar\partial/\partial x$. The complex conjugate of the operator is $p_x^* = -p_x = i\hbar\partial/\partial x$. The transpose operator is: $p_x^T = -p_x = i\hbar\nabla$. The Hermitian conjugate is then: $p_x^\dagger = (p_x^T)^* = p_x$; the momentum operator is Hermitian and therefore a good operator in quantum mechanics. ■

Another important property of Hermitian operator, that we will give here omitting the demonstration, is that all its eigenfunctions are orthogonal.

The product between two operators is trivially defined as:

$$fg\psi = f(g\psi). \tag{9}$$

Generally speaking fg and gf are different operators. It is thus useful to define the commutator between two operators as:

$$[f, g]\psi = f(g\psi) - g(f\psi). \qquad \forall\psi \tag{10}$$

If $[f, g] = 0$, the two operators are commutative.

3.c Example

The operator momentum and position are in general not commutative. As an example, let us assume a one-dimensional system. In this case, $p_x = -i\hbar\partial/\partial x$.

$$[x, p_x]\psi = x(p_x\psi) - p_x(x\psi) = -i\hbar x\frac{\partial\psi}{\partial x} + i\hbar\frac{\partial}{\partial x}(xf) = -i\hbar x\frac{\partial\psi}{\partial x} + i\hbar\psi + i\hbar x\frac{\partial\psi}{\partial x} = i\hbar\psi. \quad (11)$$

It thus follows that $[x, p_x] = i\hbar$. It is interesting to note that the operators position and momentum on different axis are commutative.We can thus generalise this example by writing: $[x_i, p_j] = \delta_{i,j}i\hbar$. (we recall here that δ_{ij} is the Kronecker function: $\delta_{ij} = 1$ if $i = j$, zero otherwise) ■

An important theorem in Quantum mechanics states that if two operators are commutative, we can always find an orthonormal and complete set of wavefunctions that are eigenvectors for both. This implies that two commutative operators represent dynamic variables that can be measured simultaneously with infinitely accurate precision. We can extend this notion by stating that for any quantum system there exists a maximum set of observables, i.e. a maximum ensemble of all the operators that are commutative among each other. If the eigenvalues of all these operators are known, the system is univocally determined.

We will conclude this lecture by reformulating a more rigorous version of the Heisenberg's uncertainty principle. Generally speaking this principle states that two conjugated variables cannot be simultaneously measured with infinite precision or, mathematically:

$$\Delta x \Delta p_x \geq \hbar/2, \quad (12)$$

with x and p_x being two general conjugated variables (position and momentum in this case). In light of what said about commutators, we can extend this formulation to:

$$\Delta A \Delta B \geq \frac{[A, B]}{2}, \quad (13)$$

with A and B being two general operators. We can see from this formulation that if two variables are conjugated they do not commute (i.e. $[A, B] \neq 0$) and, therefore, they cannot be precisely determined simultaneously. Conversely, two non-conjugated variables do commute and can be determined with an arbitrarily small accuracy.