1 Multiple Compatible Operators

Since operators are represented as matrices, the product of two operators isn't necessarily commutative, i. e., in general $AB \neq BA$. The *commutator* of two operators is defined as

$$[A, B] \equiv AB - BA. \tag{1}$$

If two operators commute, i. e., if $[A, B] = 0$, then they share eigenvectors. This is easy to show: If $A\psi = a\psi$ where A is an operator, then ψ is an eigenvector of A with eigenvalue a. Note that $AB\psi = BA\psi = Ba\psi = aB\psi$. If we write $\phi = B\psi$, then $A\phi = a\phi$. In other words, both ψ and ϕ are eigenvectors of the operator A with the same eigenvalue, a. If there is no degeneracy, then ψ and ϕ are parallel, i. e., $\phi = b\psi$, where b is just a number. However, recalling that $\phi = B\psi$, we see that $B\psi = b\psi$, and ψ is also an eigenvector of B.

If degeneracy exists such that multiple eigenvectors of A have the same eigenvalue a, then one cannot immediately infer that ϕ is parallel to ψ. However, all is not lost. If there are N eigenvectors of A, ψ_i, $i = 1, \ldots n$, then each of the N $\phi_i = B\psi_i$ can be constructed as a linear superposition of the ψ_i. This is easily shown since $A\phi_i = AB\psi_i = BA\psi_i = Ba\psi_i = aB\psi_i = a\phi_i$, implying that each of the ϕ_i is itself an eigenvector of A. However, any eigenvectors of A with eigenvalue a, including the ϕ_i, can be constructed as linear superpositions of the ψ_i. All that remains is to solve the restricted eigenvalue problem $B\chi = b\chi$, where χ is an arbitrary linear superposition of the ψ_i. There will in general be N such eigenvectors, χ_i, $i = 1, \ldots N$, with associated eigenvalues b_i. The χ_i are eigenvectors of both A and B, and the theorem is proved for the degenerate case.

The following is also true: If all eigenvectors of A are eigenvectors of B, and if all eigenvectors of B are eigenvectors of A, then $[A, B] = 0$. (See if you can show this!)

Two or more operators that mutually commute are said to be *compatible*. A quantum mechanical system becomes completely specified when all operators compatible with the Hamiltonian and with each other are found.

1.1 Position and Momentum

The position operator is just x, while the momentum operator is

$$p = -i\hbar \frac{\partial}{\partial x}. \tag{2}$$

Applying xp and px to an arbitrary function $\psi(x)$ results in

$$xp\psi = -i\hbar x \frac{\partial \psi}{\partial x} \qquad px\psi = -i\hbar \frac{\partial}{\partial x}(x\psi) = -i\hbar\psi - i\hbar x \frac{\partial \psi}{\partial x}, \tag{3}$$

so that $[x,p]\psi = i\hbar\psi$. Since this is true for any ψ, we infer that

$$[x,p] = i\hbar, \tag{4}$$

and x and p are incompatible operators.

If operators are incompatible, then exact simultaneous measurements of the corresponding physical quantities are impossible. This is because a measurement of a quantity exhibits no quantum mechanical uncertainty only when the state vector of the system is an eigenvector of the operator in question. If two operators are incompatible, then if the state vector is an eigenvector of the first operator, it cannot be an eigenvector of the second operator. The value of the physical variable associated with the second operator is thus uncertain. This is the origin of the *uncertainty principle*, which states (among other things) that the position and the momentum of a particle cannot be simultaneously measured with infinite accuracy.

1.2 Energy and Momentum of a Free Particle

The Hamiltonian of a free particle is just

$$H = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \tag{5}$$

Applying pH to an arbitrary function results in

$$pH\psi = i\frac{\hbar^3}{2m}\frac{\partial^3 \psi}{\partial x^3}. \tag{6}$$

However, application of Hp to ψ yields the same result. Thus, $[H,p] = 0$, and the Hamiltonian and momentum operators are compatible.

Eigenvectors of the free particle Hamiltonian can be obtained by solving the equation

$$H\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi, \tag{7}$$

where E is the particle energy. There are two solutions to this equation for each value of E:

$$\psi_{1,2} = \exp[\pm i(2mE)^{1/2}x/\hbar - iEt/\hbar]. \tag{8}$$

The Hamiltonian is thus degenerate. However, these solutions are also eigenvectors of the momentum operator, with the momentum eigenvalue being $+(2mE)^{1/2}$ in the first case and $-(2mE)^{1/2}$ in the second.

Alternate solutions to equation (7) are

$$\begin{aligned} \psi_a &= \cos[(2mE)^{1/2}x/\hbar]\exp(-iEt/\hbar) \\ \psi_b &= \sin[(2mE)^{1/2}x/\hbar]\exp(-iEt/\hbar). \end{aligned} \tag{9}$$

These can be obtained as a linear combination of the solutions given by equation (8) since $\cos(a) = [\exp(ia) + \exp(-ia)]/2$, etc. However, notice that these solutions are *not* eigenvectors of the momentum operator since $p\psi_a \neq const \times \psi_a$ and $p\psi_b \neq const \times \psi_b$. The actual relationships in this case are $p\psi_a = -(2mE)^{1/2}\psi_b$ and $p\psi_b = (2mE)^{1/2}\psi_a$.

1.3 Parity and Energy

The parity operator makes the transformation $x \rightarrow -x$. If, for example, x takes on the possible values $-1, 0, 1$, then the parity operator P takes the form

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{10}$$

If we have a state vector

$$\psi = \begin{pmatrix} \psi(-1) \\ \psi(0) \\ \psi(1) \end{pmatrix}, \tag{11}$$

then

$$P\psi = \begin{pmatrix} \psi(1) \\ \psi(0) \\ \psi(-1) \end{pmatrix}. \tag{12}$$

Generalization to more x values is clear.

Notice that application of the parity operator twice yields the identity operation, i. e., $P^2 = I$. The only possible eigenvalues of the parity operator are thus ± 1. In general this means that the parity operator is extremely degenerate, with many eigenvectors for each of these eigenvalues. In fact, all even functions of x are eigenvectors with eigenvalue $+1$, while all odd functions of x are eigenvectors with eigenvalue -1. The former are said to have *even parity*, while the later have *odd parity*.

The parity operator commutes with the Hamiltonian for the free particle. This may be shown as follows:

$$PH\psi(x) = P\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\right] = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial(-x)^2}. \tag{13}$$

However,

$$HP\psi(x) = H\psi(-x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(-x)}{\partial(-x)^2}, \tag{14}$$

where the chain rule operation $\partial\psi(-x)/\partial x = -\partial\psi(-x)/\partial(-x)$ has been invoked twice.

Notice that whereas $\psi_{1,2}$ in equation (8) are eigenvectors of the momentum operator, the alternate solutions to the free particle problem, $\psi_{a,b}$, defined in equation (9), are eigenvectors of the parity operator, with ψ_a having even parity and ψ_b having odd parity.

1.4 Parity and Momentum

The parity and momentum operators do not commute. In particular it is easy to show that

$$Pp\psi(x) = +i\hbar\frac{\partial\psi(-x)}{\partial(-x)} \qquad pP\psi(x) = -i\hbar\frac{\partial\psi(-x)}{\partial(-x)}, \tag{15}$$

which means that parity and momentum are incompatible operators. Thus, parity, momentum, and the free particle Hamiltonian are jointly incompatible even though the Hamiltonian is individually compatible with both. This is an example of *alternate incompatible representations* of the state of a system. We will encounter other examples of this situation as we learn more about quantum mechanics.

1.5 Generalized Uncertainty Relations

We showed that operators are compatible if they commute. In this section we show that the observables associated with two non-commuting operators cannot be simultaneously measured to arbitrary accurary.

Suppose ψ is the state vector of some system while A and B are Hermitian operators associated with measurable variables on the system. We wish to compute the RMS uncertainty in the expectation values of the two variables, $\sigma_A^2 =< (A- < A >)^2 >$, $\sigma_B^2 =< (B- < B >)^2 >$. Without loss of generality we can set $< A >= 0$ and $< B >= 0$ for any case simply by redefining the origin of the coordinate system for each variable. Let us assume that this has been done for both variables, so that $\sigma_A^2 =< A^2 >$ and $\sigma_B^2 =< B^2 >$.

Let us now define two auxiliary vectors, $\chi_A = A\psi$ and $\chi_B = B\psi$. The *Schwartz inequality* states that

$$(\chi_A, \chi_A)(\chi_B, \chi_B) \geq |(\chi_A, \chi_B)|^2. \tag{16}$$

For vectors in three-dimensional space this just states that the square of the dot product of two vectors $(\mathbf{A}\cdot\mathbf{B})^2$ is less than the product of the magnitudes of the vectors $|\mathbf{A}||\mathbf{B}|$. However, the dot product is just $|\mathbf{A}||\mathbf{B}|\cos\alpha$ where α is the angle between the vectors, so the Schwartz inequality is simply equivalent to stating that the cosine is less than or equal to unity in three-dimensional space.

We now make the following manipulations starting with the Schwartz inequality applied to the Hilbert space vectors χ_A and χ_B:

$$\begin{aligned}
(\chi_A, \chi_A)(\chi_B, \chi_B) &\geq |(\chi_A, \chi_B)|^2 \\
(A\psi, A\psi)(B\psi, B\psi) &\geq |(A\psi, B\psi)|^2 \\
(\psi, A^2\psi)(\psi, B^2\psi) &\geq |(\psi, AB\psi)|^2,
\end{aligned} \tag{17}$$

where the last step works because A and B are Hermitian. We now note that these dot products are in the form of expectation values, so we continue as follows:

$$\begin{aligned}
| < AB > |^2 &= | < AB + BA > /2+ < AB - BA > /2|^2 \\
&= | < AB + BA > + < [A, B] > |^2/4 \\
&\geq | < [A, B] > |^2/4.
\end{aligned} \tag{18}$$

The last step depends on the following argument: The operator $AB + BA$ is Hermitian, and so produces real expectation values. The expectation value $< AB + BA >$ is therefore real. However, the operator $[A, B]$ is anti-Hermitian, i. e., $[A, B]' = (AB)' - (BA)' = B'A' - A'B' = BA - AB = -[A, B]$, so it produces imaginary expectation values. Thus, $| < AB + BA > /2 + < AB - BA > /2|^2$ is in the form $|\alpha + i\beta|^2 = \alpha^2 + \beta^2$, where α and β are real. However, $\alpha^2 + \beta^2 \geq \beta^2$.

Taking the square root of the above result shows that

$$\sigma_A \sigma_B \geq | < [A, B] > |/2. \tag{19}$$

Thus, the product of the uncertainties in the expectation values of A and B is at a minimum half the expectation value of the commutator of A and B. If the commutator is non-zero, the uncertainty in the two variables cannot be simulaneously reduced to zero.

Let us apply this to the position and momentum operators, $A = x$ and $B = -i\hbar\partial/\partial x$. We find that

$$< [x, p] >= i\hbar. \tag{20}$$

Thus, we have

$$\sigma_x \sigma_p \geq \hbar/2. \tag{21}$$

This is a precise expression of the well-known uncertainty relationship between position and momentum.