Operator Methods

The quantum mechanics we've encountered so far has been expressed in terms of wavefunctions. We will reformulate it in terms of **operators** acting on **states**, as opposed to acting on wavefunctions. This turns out to be elegant, compact and powerful for quantum mechanical calculations. For example, the energy spectrum of the quantum harmonic oscillator can be found without the need for solving differential equations; see Section 5. In Sections 1 to 4, we begin with the mathematical definitions that underpin this approach: however, on a first reading the reader may wish to jump directly to Section 5.

1 Quantum mechanical states

A general quantum mechanical state can be described by a **state vector** or 'ket', $|\psi\rangle$. A ket contains all information about that specific state. For each state vector, a corresponding **dual state vector** is represented by the 'bra', $\langle\psi|$. This notation is known as Dirac notation. Together, bras and kets allow us to define the **overlap** ('bra-ket') between two states, $\langle\psi_1|\psi_2\rangle$, which is in general a complex number. This is analogous to the scalar product of two vectors: if the vectors are perpendicular, then the scalar product is zero, and if they are parallel it is maximum. The overlap of a quantum state with itself is defined to be positive and is frequently imposed to be unity, $\langle\psi_1|\psi_1\rangle = 1$. This condition is known as the **normalisation** of quantum states, and will be assumed from now on. When $\langle\psi_1|\psi_2\rangle = 0$ (no overlap), the states are said to be **orthogonal** to each other. In general, $0 \le |\langle\psi_1|\psi_2\rangle| \le 1$. Furthermore, we define that for any pair of states, $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$, where the superscript '$*$' denotes complex conjugation.

It is frequently helpful to express a state as a **linear combination** of other states. A set of kets $\{|\phi_n\rangle\}$ forms a **basis** if any state of the system can be expressed as a linear combination of the $\{|\phi_n\rangle\}$:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \ , \tag{1}$$

where c_n is the weight corresponding to the state $|\phi_n\rangle$. A basis is said to **span** the space where the states 'live', known as a **Hilbert space**. It is convenient to choose the basis states $\{|\phi_n\rangle\}$ such that they are **orthonormal**, a condition which can be expressed using the Kronecker delta δ_{nm}:

$$\langle\psi_n|\psi_m\rangle = \delta_{nm} \ . \tag{2}$$

2 Quantum Mechanical Operators

An **operator** is a mathematical object which acts on a state to produce another state: $\hat{O}|a\rangle = |b\rangle$. If the action of operator $\hat{O}$ on a state $|\phi\rangle$ returns the same state $|\phi\rangle$ multiplied by a constant λ,

$$\hat{O}|\phi\rangle = \lambda|\phi\rangle \ , \tag{3}$$

then $|\phi\rangle$ is said to be an **eigenstate** of $\hat{O}$ with **eigenvalue** λ.

The action of an operator $\hat{O}$ on a general state $|\psi\rangle$ can be computed by expanding $|\psi\rangle$ in terms of the eigenstates of $\hat{O}$, $\{|\phi_n\rangle\}$:

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle \ , \tag{4}$$

where the coefficients c_n are the overlaps: $c_n = \langle\phi_n|\psi\rangle$. Then:

$$\hat{O}|\psi\rangle = \sum_n c_n\hat{O}|\phi_n\rangle \ , \tag{5}$$

$$= \sum_n c_n\lambda_n|\phi_n\rangle \ , \tag{6}$$

where $\{\lambda_n\}$ is the set of eigenvalues for the eigenvectors $\{|\phi_n\rangle\}$. Physical observables, such as position and momentum, are represented by so-called *Hermitian* operators, which have real eigenvalues. The average value of the observable represented by the operator $\hat{O}$ in a state $|m\rangle$ is given by $\langle m|\hat{O}|m\rangle$: this is called the expectation value of the operator. In general, we can define **matrix elements** of an operator between any two states as $O_{mn} = \langle m|\hat{O}|n\rangle$.

3 Representations of state vectors and relation to the wavefunction

A particularly important basis is given by the eigenstates $|x\rangle$ of the position operator:

$$\hat{x}|x\rangle = x|x\rangle \ . \tag{7}$$

The position x takes continuous values, so the normalization condition is expressed with the Dirac delta function:

$$\langle x'|x\rangle = \delta(x - x') \ . \tag{8}$$

A general state $|\psi\rangle$ can be expressed as a linear combination of position eigenstates as

$$|\psi\rangle = \int dx\, |x\rangle\langle x|\psi\rangle \ . \tag{9}$$

It can be seen that the operator $\int dx\, |x\rangle\langle x| \equiv 1$ is equivalent to a **resolution of the identity**. Up to this point we have been dealing with a state vector $|\psi\rangle$ that is an element of a Hilbert space. The coordinate space wavefunction we discussed in Sheet 2 can be obtained by **projecting** this state onto the position basis:

$$\psi(x) = \langle x|\psi\rangle. \tag{10}$$

The wavefunction provides the **position representation** of the state vector. Similarly, the momentum-space wavefunction provides the **momentum representation** of the state vector:

$$\psi(p) = \langle p|\psi\rangle \ . \tag{11}$$

These equations allow us to calculate the overlap of two general states $|\psi\rangle$ and $|\phi\rangle$, for example using the position basis:

$$\langle\psi|\phi\rangle = \langle\psi|\left(\int dx|x\rangle\langle x|\phi\rangle\right) = \int dx\langle\psi|x\rangle\langle x|\phi\rangle = \int dx\psi^*(x)\phi(x) \ . \tag{12}$$

Operators can be analogously expressed in a given representation by considering their matrix element between two general states of the corresponding basis: e.g. in the position representation,

$$\langle x|\hat{x}|x'\rangle = x\delta(x-x') \qquad \langle x|\hat{p}|x'\rangle = -i\hbar\delta(x-x')\partial_x \,. \tag{13}$$

Using these relations and expressing a general state $|\psi\rangle$ in terms of the $|x\rangle$ basis, we obtain the identities:

$$\langle x|\hat{x}|\psi\rangle = x\psi(x) \,, \quad \langle x|\hat{p}|\psi\rangle = -i\hbar\partial_x\psi(x) \,. \tag{14}$$

4 Commutation Relations

Commutativity is the property that changing the order in which a set of mathematical operations (e.g. ordinary multiplication and addition) is applied does not change the final outcome. Conversely, noncommutativity occurs when the applied order changes the outcome (e.g. in general, when multiplying two matrices A and B, $AB \neq BA$). This is relevant as operators in quantum mechanics do not necessarily commute with each other. Commutativity (or the lack thereof) is quantified by the **commutator**, which for two operators A and B is defined as:

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \,. \tag{15}$$

For example, the classical position and momentum of a particle commute, $[x,p] = 0$, since x and p are just numbers. However, the quantum position and momentum operators have a non-zero commutator, given by:

$$[\hat{x},\hat{p}] = i\hbar \,. \tag{16}$$

This relation can be obtained from the action of the position representation of $\hat{x}$ and $\hat{p}$ on a general function: $[x,-i\hbar\partial_x]f(x) = i\hbar f(x)$. Notice that the commutator vanishes as $\hbar \to 0$: this is known as the **classical limit**, where we are expected to recover classical results. A commutator features in the general form of **Heisenberg's uncertainty principle**:

$$\Delta A \Delta B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle| \,, \tag{17}$$

where ΔA and ΔB are the uncertainties ($\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$) associated with the observables A and B and $\langle\dots\rangle$ denotes the expectation value.

5 The Harmonic Oscillator revisited: Creation and Annihilation Operators

To illustrate the power of operator methods, we will use them to solve the quantum harmonic oscillator problem without having to deal with differential equations. The Hamiltonian is given by:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \,. \tag{18}$$

It is tempting to try to factorize $\hat{H}$ as the product of two operators involving linear combinations of $\hat{p}$ and $\hat{x}$. To achieve this, we introduce the so-called **lowering** and **raising** operators, respectively defined as:

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) \quad , \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \,. \tag{19}$$

These are sometimes referred to as **ladder operators**, for reasons that will soon become clear. The Hamiltonian can be written in terms of the ladder operators as:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) , \tag{20}$$

where the extra factor of $\hbar\omega/2$ arises from the non-commutativity of $\hat{x}$ and $\hat{p}$. The ladder operators satisfy $[\hat{a},\hat{a}^\dagger] = 1$. In the operator framework the time-independent Schrödinger equation is,

$$\hat{H}|n\rangle = E_n|n\rangle \,. \tag{21}$$

We want to construct the eigenstates $|n\rangle$ of the Hamiltonian and compute the corresponding eigenvalues E_n. In order to do this, we need to know the action of the operators $\hat{a}$ and $\hat{a}^\dagger$ on $|n\rangle$. From the commutation relations $[\hat{H},\hat{a}] = -\hbar\omega\hat{a}$ and $[\hat{H},\hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger$, it is readily seen that:

$$\hat{H}\hat{a}^\dagger|n\rangle = (E_n + \hbar\omega)\hat{a}^\dagger|n\rangle \,, \tag{22}$$

$$\hat{H}\hat{a}|n\rangle = (E_n - \hbar\omega)\hat{a}|n\rangle \,. \tag{23}$$

It follows that $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$ are also eigenstates of the Hamiltonian with eigenvalues $E_n \pm \hbar\omega$ respectively, i.e. the raising and lowering operators raise and lower the energy by $\hbar\omega$. The spectrum of the Hamiltonian must be positive because the Hamiltonian is a sum of squares. It follows that there exists a state $|0\rangle$, the ground state, such that it is not possible to lower the energy any further, $a|0\rangle = 0$. From Eq. (20), we find that the corresponding energy is given by $E_0 = \hbar\omega/2$. Repeated application of the raising operator via Eq. (22) yields the spectrum of the quantum harmonic oscillator,

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \,, \tag{24}$$

where $n = 0,1,2,\dots$. Comparing this result with the Hamiltonian expressed in terms of the ladder operators, we see that the operator $\hat{n} \equiv \hat{a}^\dagger\hat{a}$ has eigenvalue n and it is then referred to as the **number operator**.

We have found that the action of the ladder operators on a particular eigenstate $|n\rangle$ gives another eigenstate with energy $E_n \pm \hbar\omega$. From the spectrum in Eq. (24), we see that the energy difference between $|n \pm 1\rangle$ and $|n\rangle$ is given by $\pm\hbar\omega$. Hence, $\hat{a}^\dagger|n\rangle = \mathcal{C}|n+1\rangle$ and $\hat{a}|n\rangle = \mathcal{D}|n-1\rangle$, where $\mathcal{C}$ and $\mathcal{D}$ are constants to be determined. Using the normalization condition $\langle n+1|n+1\rangle = \langle n-1|n-1\rangle = 1$ and the known action of the number operator, $\hat{n}|n\rangle = n|n\rangle$, we can determine the constants C and D as:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad , \quad \hat{a}^\dagger = \sqrt{n+1}|n+1\rangle \,. \tag{25}$$

It is now clear that any excited state can be constructed by the repeated action of $\hat{a}^\dagger$ on the ground state $|0\rangle$:

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \,, \tag{26}$$

where the factorial is required by normalization.

Using ladder operators, we have successfully determined the eigenstates and energies of the harmonic oscillator without having to solve differential equations. We have determined that the ladder operators act to raise or lower a quantum state by one level, thus changing its energy by $\pm\hbar\omega$. The state $|n\rangle$ may be regarded as having n **quanta** of energy $\hbar\omega$ above the ground state. These excitations turn out to be bosons and are created and destroyed by the ladder operators. This picture is very useful and extensively employed in more advanced quantum physics applications.