Observables as Hermitian Operators

- All observable physical quantities are represented in quantum mechanics by operators. In this tutorial we will explore some properties that these operators must have.
- Property 1: When any operator $\hat{Q}$ acts on a physical (i.e. in the Hilbert space) quantum state $|\Psi\rangle$, it produces another state vector $\hat{Q}|\Psi\rangle = |\hat{Q}\Psi\rangle$. *Most* of the time this new state vector will also be in the Hilbert space, but there are some pathological cases. If needed, we can always exclude these pathological states from the domain of our operator.
- Property 2: The expectation value of of any operator must be real.
- Show that Properties 1 and 2 imply that $\langle\Psi|\hat{Q}\Psi\rangle = \langle\hat{Q}\Psi|\Psi\rangle$.

- Operators that satisfy $\langle\Phi|\hat{Q}\Psi\rangle = \langle\hat{Q}\Phi|\Psi\rangle$ for all $|\Psi\rangle$ and $|\Phi\rangle$ in the Hilbert space are said to be *Hermitian*. Show that the operator $\hat{p} = -i\hbar d/dx$ is Hermitian by writing $\langle\Phi|\hat{p}\Psi\rangle$ as an integral. Then try to rewrite the integral to form $\langle\hat{p}\Phi|\Psi\rangle$. (Hint: use integration by parts.)

- Now suppose we choose to represent our quantum states in a complete basis with discrete basis vectors $|n\rangle$ (so there are as many basis vectors as whole numbers). Then we can write the right vector for our quantum state as

$$|\Psi\rangle = \sum_n c_n |n\rangle$$

and the left vector for the same state as

$$\langle\Psi| = \sum_m c_m^* \langle m|.$$

Use this basis to write the expectation value $\langle\hat{Q}\rangle$.

- Let's define $Q_{mn} = \langle m|\hat{Q}|n\rangle$. Rewrite the expectation value $\langle\hat{Q}\rangle$ using this definition. Show that the result is equivalent to multiplying a column vector with components c_n by a matrix with elements Q_{mn} and then multiplying that result by a row vector with components c_m^*.

- Show that if $\hat{Q}$ is Hermitian then $Q_{nm}^* = Q_{mn}$. (Note: we define the *Hermitian conjugate* $\hat{Q}^\dagger$ of a matrix as $Q_{mn}^\dagger = Q_{nm}^*$. Then $\hat{Q}^\dagger = \hat{Q}$ if $\hat{Q}$ is a Hermitian matrix/operator.)

- Suppose our basis vectors $|n\rangle$ are eigenstates of the operator $\hat{Q}$ so that $\hat{Q}|n\rangle = q_n|n\rangle$. Evaluate $\langle\hat{Q}\rangle$ for the state $|\Psi\rangle = \sum_n c_n|n\rangle$. (Note: you will need to start with a double sum, but you should be able to reduce to a single sum.) The set of eigenvalues q_n of an operator $\hat{Q}$ is known as the *spectrum* of $\hat{Q}$. This is related to the spectrum of light emitted by a gas, but it's not quite the same.

- What is the expectation value for $\hat{Q}$ when the quantum state is $|n\rangle$?

- What is the expectation value for $\hat{Q}^2$ when the quantum state is $|n\rangle$?

- Calculate the standard deviation σ_Q for the state $|n\rangle$. What does this result tell you about the state $|n\rangle$?

- Show that the eigenvalues q_n must be real by evaluating $\langle n|\hat{Q}n\rangle$ and $\langle\hat{Q}n|n\rangle$ and using the fact that $\hat{Q}$ is Hermitian.

- Show that two eigenstates $|n\rangle$ and $|m\rangle$ with distinct real eigenvalues, q_n and q_m, are orthogonal to each other. Evaluate $\langle m|\hat{Q}n\rangle$ and $\langle \hat{Q}m|n\rangle$ and use the fact that $\hat{Q}$ is Hermitian.

- Note that two eigenstates that have the same eigenvalue (a situation called *degenerate* eigenvalues) are not necessarily orthogonal. However, they can be made orthogonal using the *Gram-Schmidt procedure.* Consider two vectors:
$$|f\rangle = \begin{pmatrix} 3 \\ -4 \end{pmatrix}, \qquad\qquad |g\rangle = \begin{pmatrix} 2 \\ 1 \end{pmatrix}.$$
Find a unit vector $|f'\rangle$ that is parallel to $|f\rangle$.

- Compute the inner product $\langle f'|g\rangle$.

- Find the vector $|h\rangle = |g\rangle - \langle f'|g\rangle|f'\rangle$.

- Find the unit vector $|h'\rangle$ that is parallel to $|h\rangle$.

- Show that $|f'\rangle$ and $|h'\rangle$ are orthogonal.

- Note that if $f\rangle$ and $|g\rangle$ were eigenstates of $\hat{O}$ with the same eigenvalue q, then $|f'\rangle$ and $|h'\rangle$ are also eigenstates of $\hat{O}$, both with eigenvalue q. Therefore the eigenstates of a Hermitian operator can be made to form a complete set of orthonormal basis vectors.