Intermediate Quantum Mechanics
Lecture 3 Notes (1/28/15)

Linear Operators, Postulates of QM

Completeness Relation

- Any vector can be expressed as a linear superposition of a set of basis vectors.

$$|a\rangle \;=\; a_1\,|1\rangle \;+\; a_2\,|2\rangle \;+\; \cdots \;+\; a_n\,|n\rangle \;=\; \sum_i a_i\,|i\rangle$$

- Using the fact that the basis vectors are orthonormal:

$$\langle i\,|\,j\,\rangle \;=\; \delta_{ij}$$

  we find that the components of $|a\rangle$ are given by its projection onto the basis vectors:

$$\langle j\,|\,a\,\rangle \;=\; \sum_i a_i\,\langle j\,|\,i\,\rangle \;=\; a_j$$

- Now substitute into the above equation for $|a\rangle$:

$$|a\rangle \;=\; \sum_i a_i\,|i\rangle \;=\; \sum_i \langle i\,|\,a\,\rangle\,|i\rangle \;=\; \sum_i\,|i\rangle\,\langle i\,|\,a\,\rangle \;=\; \left(\sum_i\,|i\rangle\langle i|\right)\,|a\rangle$$

- The expression $\sum_i |i\rangle\langle i|$ doesn't do anything. It just leaves the vector $|a\rangle$ as it is. It is the identity operator:

$$\sum_i\,|i\rangle\langle i| \;=\; \hat{I} \;\Longrightarrow\; \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & 1 \end{pmatrix}$$

- This is called the **Completeness Relation**. Note that in order for it to be the identity operator the sum must be over <u>all</u> of the basis vectors. If just over one basis vector, it will be the projection of $|a\rangle$ on that basis vector, $\langle i\,|\,a\,\rangle\,|i\rangle$. If over two basis vectors, it will be the projection of $|a\rangle$ onto the plane spanned by the two basis vectors, $\langle i\,|\,a\,\rangle\,|i\rangle \;+\; \langle j\,|\,a\,\rangle\,|j\rangle$, and so on. Projection operators are an important tool that we discuss and use later.

- The importance of the completeness relation is that, since it is the identity operator, we can stick it wherever we like into any vector expression.

Linear Operators

- An **operator** acts on a vector yielding another (or the same) vector. An operator $\hat{M}$ acting on $|a\rangle$ is:

$$\hat{M}\,|a\rangle \;=\; |b\rangle$$

- In quantum mechanics, all operators are **linear operators**. That means:

$$\hat{M}\big(\alpha\,|a\rangle \;+\; \beta\,|b\rangle\big) \;=\; \alpha\hat{M}\,|a\rangle \;+\; \beta\hat{M}\,|b\rangle$$

Matrix Representation of Operators

- In a given basis, an operator is represented by a square matrix. Here we use the completeness relation to write:

$$|b\rangle \;=\; \hat{M}\,|a\rangle \;=\; \sum_j \hat{M}\,|j\rangle\,\langle j\,|\,a\,\rangle$$

$$\langle i\,|\,b\,\rangle \;=\; \langle i|\hat{M}\,|a\rangle \;=\; \sum_j \langle i|\hat{M}\,|j\rangle\,\langle j\,|\,a\,\rangle$$

This is of the form of (a vector component of $|b\rangle$) equals (the vector components of $|a\rangle$) multiplied by (a matrix representing the operator $\hat{M}$).

$$|b\rangle \;=\; \hat{M}\,|a\rangle$$

$$\Longrightarrow \qquad \begin{pmatrix} \langle 1\,|\,b\,\rangle \\ \langle 2\,|\,b\,\rangle \\ \cdot \\ \cdot \\ \cdot \\ \langle n\,|\,b\,\rangle \end{pmatrix} = \begin{pmatrix} \langle 1|\hat{M}\,|1\rangle & \langle 1|\hat{M}\,|2\rangle & \cdot & \cdot & \cdot & \langle 1|\hat{M}\,|n\rangle \\ \langle 2|\hat{M}\,|1\rangle & \langle 2|\hat{M}\,|2\rangle & \cdot & \cdot & \cdot & \langle 2|\hat{M}\,|n\rangle \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \langle n|\hat{M}\,|1\rangle & \langle n|\hat{M}\,|2\rangle & \cdot & \cdot & \cdot & \langle n|\hat{M}\,|n\rangle \end{pmatrix} \begin{pmatrix} \langle 1\,|\,a\,\rangle \\ \langle 2\,|\,a\,\rangle \\ \cdot \\ \cdot \\ \cdot \\ \langle n\,|\,a\,\rangle \end{pmatrix}$$

$$= \begin{pmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_n \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} & \cdot & \cdot & \cdot & m_{1n} \\ m_{21} & m_{22} & \cdot & \cdot & \cdot & m_{2n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ m_{n1} & m_{n2} & \cdot & \cdot & \cdot & m_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{pmatrix}$$

$\langle i|\hat{M}\,|j\rangle$ are the matrix elements m_{ij} of the matrix representing $\hat{M}$ in the $|i\rangle$, $|j\rangle$ basis.

- A 2-dimensional example:

$$a_j \;=\; \langle j\,|\,a\,\rangle \qquad b_i \;=\; \langle i\,|\,b\,\rangle \qquad m_{ij} \;=\; \langle i|\hat{M}\,|j\rangle$$

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$$b_1 \;=\; m_{11}a_1 \;+\; m_{12}a_2 \qquad\qquad b_2 \;=\; m_{21}a_1 \;+\; m_{22}a_2$$

- Physicists don't always use precise language. The quantity $\langle a|\hat{M}\,|b\rangle$ is usually referred to as the matrix element of a with b. Of course, it's only really a matrix element in the basis in which $|a\rangle$ and $|b\rangle$ are basis vectors. For the 2-dimensional case, the expression for $\langle a|\hat{M}\,|b\rangle$ is obtained from:

$$\langle a|\hat{M}\,|b\rangle \;=\; (a_1^*, a_2^*)\begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

I'll ask you to work that out in a homework problem just to give an exercise in matrix multiplication.

Eigenvalues and Eigenvectors

- If $\hat{M}$ operating on a vector gives a number times that vector:

$$\hat{M}\,|a\rangle \;=\; \lambda_a\,|a\rangle$$

we call $|a\rangle$ an **eigenvector** of $\hat{M}$ and the (complex) number λ_a the corresponding **eigenvalue**.

- The eigenvalues are the diagonal elements of the matrix in the representation in which the matrix is diagonalized (has only diagonal elements). Not all operators can be diagonalized and, therefore, not all operators have eigenvectors.

Hermitian Conjugate

- For operators in complex vectors spaces, we need to have the concept of the conjugation of an operator. The Hermitian conjugate of an operator $\hat{M}$ is labeled $\hat{M}^\dagger$ and is defined by:

$$\langle a|\hat{M}^\dagger\,|b\rangle \;=\; \langle b|\hat{M}\,|a\rangle^*$$

- From this we get the relation between the matrix elements of $\hat{M}^\dagger$ and $\hat{M}$.

$$\langle b|\hat{M}\,|a\rangle \;=\; \sum_i \langle b|\hat{M}\,|i\rangle\,\langle\, i\,|\,a\,\rangle \;=\; \sum_{i,j}\langle\, b\,|\,j\,\rangle\langle j|\hat{M}\,|i\rangle\,\langle\, i\,|\,a\,\rangle \;=\; \sum_{i,j} b_j^*\,m_{ji}\,a_i$$

$$\Rightarrow\;\; \langle b|\hat{M}\,|a\rangle^* \;=\; \sum_{i,j} b_j\,m_{ji}^*\,a_i^* \;=\; \sum_{i,j} a_i^*\,m_{ji}^*\,b_j \;=\; \sum_{i,j} a_i^*\,m_{ij}^\dagger\,b_j \;=\; \langle a|\hat{M}^\dagger\,|b\rangle$$

$$\Rightarrow \qquad m_{ij}^\dagger \;=\; m_{ji}^*$$

The matrix elements of the Hermitian conjugate of $\hat{M}$ are obtained by transposing (interchanging rows and columns) and complex conjugating the matrix elements of $\hat{M}$.

$$\hat{M} \;\Longrightarrow\; \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \qquad\qquad \hat{M}^\dagger \;\Longrightarrow\; \begin{pmatrix} m_{11}^* & m_{21}^* \\ m_{12}^* & m_{22}^* \end{pmatrix}$$

- In the case of a real operator, the Hermitian conjugate is just the transpose operator. $\hat{M}^\dagger \;=\; \hat{M}^T$

Hermitian Operator

- Hermitian operators play a central role in quantum mechanics.
- A Hermitian operator, $\hat{\mathcal{H}}$, is defined as an operator that is equal to its Hermitian conjugate.

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}^\dagger \qquad \Rightarrow \qquad h_{ij} = h_{ij}^\dagger = h_{ji}^*$$

- Clearly the diagonal matrix elements of a Hermitian operator are real and in general:

$$\langle a|\hat{\mathcal{H}}\,|b\rangle^* = \langle b|\hat{\mathcal{H}}^\dagger\,|a\rangle = \langle b|\hat{\mathcal{H}}\,|a\rangle$$

- A real Hermitian operator is a symmetric operator: $h_{ji} = h_{ij}$.

Theorems of Hermitian Operators

1) **The number of eigenvalues and the number of distinct eigenvectors of a Hermitian operator are equal to the number of dimensions of the vector space.**

   This is not too hard to prove but requires using the characteristic equation. I don't want to spend tie on that. If you are interested you can prove it for yourself or you can find it discussed in a textbook such as the Principles of Quantum Mechanics by R. Shankar pp. 32-37.

2) **All eigenvalues of a Hermitian operator are real.**

   This is easy to prove and is assigned as a homework problem.

3) **Eigenvectors of a Hermitian operator that have unequal eigenvalues are mutually orthogonal. If $\lambda_a \neq \lambda_b$ then $\langle a\,|\,b\,\rangle = 0$.**

   This is easy to prove and is assigned as a homework problem.

3′) **Linear combinations of eigenvectors of a Hermitian operator with equal eigenvalues can be found that are mutually orthogonal.**

   This can be shown by using the Gram-Schmidt procedure. See the addendum at the end of these notes.

4) **The eigenvectors of a Hermitian operator form a complete set of mutually orthogonal vectors that, when properly normalized, are a set of basis vectors for the space.**

   This follows directly from Theorems 1), 3) and 3′) above.

The Postulates of Quantum Mechanics

- We are now ready to give the complete theory of quantum mechanics in the form of six postulates.

  Postulate 1

  The possible states of a system are elements of a complex vector space.

  Postulate 2

  Observables (quantities that can be measured) correspond to Hermitian operators. There is a one-to-one correspondence between observables and Hermitian operators, the only exception being the identity operator.

Postulate 3

The only possible values of an observable are the eigenvalues of the corresponding Hermitian operator.

Postulate 4

For a state $|\psi\rangle$, the probability of measuring an observable with value λ_a is:

$$\text{Prob}(\lambda_a) \;=\; |\langle a \,|\, \psi \rangle|^2 \;=\; \langle \psi \,|\, a \rangle \langle a \,|\, \psi \rangle$$

where $|a\rangle$ is an eigenvector of the corresponding Hermitian operator with eigenvalue λ_a.

Postulate 4′

Eigenvectors are states for which the observable have a definite value with no uncertainty.

Postulate 5

When an observable is measured, the system is left in the state that is the eigenvector whose eigenvalue is the value measured.

Postulate 6

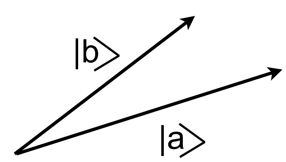
The evolution of the state of a system in time is given by:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle \;=\; \hat{H} \; |\psi(t)\rangle$$

where $\hat{H}$ is the Hermitian operator corresponding to the energy observable. It is called the Hamiltonian.

Addendum on the Gram-Schmidt Procedure

- The Gram-Schmidt procedure is a cookbook method for finding orthonormal vectors.
- Consider two linear independent vectors $|a\rangle$ and $|b\rangle$. From these, we will construct two orthonormal vectors $|\alpha\rangle$ and $|\beta\rangle$.



Step 1: Arbitrarily choose $|a\rangle$ and normalize it to get $|\alpha\rangle$.

$$|\alpha\rangle \;=\; \frac{|a\rangle}{\sqrt{\langle a \,|\, a \rangle}}$$

Step 2: Subtract from $|b\rangle$ the projection of $|b\rangle$ onto $|\alpha\rangle$.

$$|b'\rangle \;=\; |b\rangle \;-\; \langle \alpha \,|\, b \rangle \, |\alpha\rangle$$

Step 3: Normalize $|b'\rangle$ to get $|\beta\rangle$.

$$|\beta\rangle \;=\; \frac{|b'\rangle}{\sqrt{\langle b' \,|\, b' \rangle}}$$

If we were given there linearly independent vectors $|a\rangle$, $|b\rangle$ and $|c\rangle$ and were to construct from these three orthonormal vectors $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$, we would proceed as above to get $|\alpha\rangle$ and $|\beta\rangle$. Then, $|c'\rangle$ would be obtained by subtracting from $|c\rangle$ the projection of $|c\rangle$ onto the plane spanned by $|\alpha\rangle$ and $|\beta\rangle$.

$$|c'\rangle \;=\; |c\rangle \;-\; \langle \alpha \,|\, c \,\rangle\, |\alpha\rangle \;-\; \langle \beta \,|\, c \,\rangle\, |\beta\rangle$$

Then, normalize $|c'\rangle$ to get $|\gamma\rangle$.

$$|\gamma\rangle \;=\; \frac{|c'\rangle}{\sqrt{\langle c' \,|\, c' \,\rangle}}$$