1 Observables, Operators, and State Vectors

We have learned that the expectation value of the wavenumber from a wave function of the form

$$\psi = \sum_i \phi_i \exp(ik_i x), \qquad \sum_i |\phi_i|^2 = 1, \tag{1}$$

is

$$< k >= \sum_i \phi_i^* k_i \phi_i. \tag{2}$$

If we evaluate x at intervals of Δx over the domain $[-L/2, L/2]$ where $L = M\Delta x$, let the wavenumber take on the possible values $k_j = 2\pi j/L$ where $-M/2 + 1 \leq j \leq M/2$, and normalize ψ, then equation (1) becomes just an inverse finite Fourier transform:

$$\psi_m = \frac{1}{\sqrt{M}} \sum_n \phi_n \exp(i2\pi nm/M). \tag{3}$$

The corresponding forward transform is

$$\phi_n = \frac{1}{\sqrt{M}} \sum_m \psi_m \exp(-i2\pi mn/M). \tag{4}$$

Writing $q_{mn} = \exp(-i2\pi mn/M)/\sqrt{M}$, the above two equations can be written compactly as $\phi = q\psi$ and $\psi = q'\phi$. The matrix q is unitary since $\psi = q'q\psi$ and $\phi = qq'\phi$, which shows that $qq' = q'q = I$, I being the identity matrix.

We interpret the ψ_i and the ϕ_i as being the components of a single vector called the *state vector*, resolved in two different coordinate systems. The state vector is thus an abstraction which is independent of coordinate system in the same way that an ordinary vector is an abstract way of representing a direction and magnitude in three-dimensional space. Resolve the state vector in one coordinate system and the components are the amplitudes for finding a particle at each possible location. Resolve it in another coordinate system and the components represent the amplitudes associated with each possible value of wavenumber or momentum. It is possible to obtain the components in one coordinate system from those in another coordinate system by a unitary transformation, as illustrated in the above example.

All the information that is knowable about a particle is contained in the state vector. This is the central abstraction of modern quantum mechanics and it paves the way for the use of linear algebra as the "gears and levers" of quantum mechanical theory.

The formula for the expectation value can be written in the notation of linear algebra. For example,

$$< x >= \sum_i \psi_i^* x_i \psi_i = \sum_{i,j} \psi_i^* x_i \delta_{ij} \psi_j, \tag{5}$$

where δ_{ij} is the Kronecker delta. Think of the quantity $x_i \delta_{ij}$ as a diagonal matrix with the possible values of x lined up along the diagonal, while ψ_j is a column vector. The row vector ψ_i^* is the adjoint (i. e., the complex conjugate transpose) of ψ_i. In the notation of the dot product in Hilbert space,

$$< x >= (\psi, x\psi), \tag{6}$$

where x in this equation is the above-described matrix.

Suppose we have the x_i components of the state vector, ψ_i, and we wish to obtain the expectation value of the wavenumber. How do we proceed? One way is to transform to the momentum components of the state vector using a unitary transformation: $\phi = q\psi$. From this we can directly compute the expectation value of the wavenumber: $< k >= (\phi, k\phi)$, where the k in this formula is the matrix with the k_i along the diagonal. However, we can also write $< k >$ directly in terms of ψ:

$$< k >= (\phi, k\phi) = (q\psi, kq\psi) = (\psi, q'kq\psi). \tag{7}$$

The matrix $q'kq$ is no longer diagonal, and thus the calculation of the expectation value is somewhat more tedious. However, this technique does allow the direct computation of the expectation value of a variable from the components of the state vector projected onto *any* coordinate system, provided that the unitary transformation from the natural coordinate system for that variable to the new coordinate system is known. From our knowledge of linear algebra, we know that the natural coordinate system for a particular variable is called the *principal axis* coordinate system.

Just as we abstract the notion of a vector from the idea of a quantity with magnitude and direction, we develop the idea of an *operator* as a coordinate-system-independent abstraction. If the components of a matrix A which represent an operator in a particular coordinate system are known, then the components in some new coordinate system are given by qAq', where

q is the unitary transformation from the old to the new coordinate system. (Note that the old coordinate system in equation (7) is the wavenumber representation while the new system is the physical space representation, which means that the transformation matrix is actually q'.) We further simplify the notation and implicitly assume that the matrix representing the operator has been transformed into the coordinate system in which the state vector is resolved, allowing us to dispense with the qs. Thus, the expectation value for A becomes symbolically

$$< A >= (\psi, A\psi) \tag{8}$$

regardless of the coordinate system being used. The use of the same symbol for the observable, the expectation value, and the operator generally causes no confusion because the three uses can be told apart by context.

Operators representing physically observable quantities are *self-adjoint* or *Hermitian*, which means that $A_{ij} = A_{ji}^*$ where A_{ij} is the i-jth matrix component for the operator A resolved in some coordinate system. This is manifestly true in the natural or principal axis coordinate system of the operator — off-diagonal terms are zero and self-adjointness means that diagonal terms are real — a necessary condition if they are values of some observable quantity. If the matrix of an operator is self-adjoint in one coordinate system, including the principal axis system, it is self-adjoint in all, which means that this is a property of the operator itself and not just the matrices representing it in different coordinate systems.

One way of characterizing an operator is that multiplying it with any vector produces some other vector. This is evident from the matrix representation of operators. Multiplying a column matrix (the vector) by a square matrix (the operator) results in another column matrix or vector.

So far we have considered the problem of starting with an operator in its principal axis representation and finding other representations. The usual problem in quantum mechanics is the reverse — given the representation of an operator in some arbitrary coordinate system, find the representation in the principal axis system and the unitary transformation that sends the operator into this system from the original representation.

Dotting a coordinate axis unit vector of the principal axis frame with an operator yields the unit vector back again multiplied by the corresponding value on the diagonal of the operator matrix. For instance,

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 3 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}. \tag{9}$$

The coordinate axis unit vectors in the principal axis frame are called *eigenvectors*, and the values along the diagonal of the matrix are called *eigenvalues*. Each eigenvalue has an associated eigenvector.

The relationship between operators and their eigenvectors holds in all reference frames. Thus, a logical way to look for the eigenvectors and eigenvalues of an operator A is to try to solve the equation

$$A\psi = a\psi, \tag{10}$$

where ψ is the eigenvector to be deduced and a is its associated eigenvalue.

A three-dimensional example suffices to illustrate the technique, at least in principle. The equation

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = a \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} \tag{11}$$

can be written

$$\begin{pmatrix} A_{11} - a & A_{12} & A_{13} \\ A_{21} & A_{22} - a & A_{23} \\ A_{31} & A_{32} & A_{33} - a \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = 0. \tag{12}$$

This equation only has non-trivial solutions for the ψ_i if the determinant of the matrix is zero:

$$\begin{vmatrix} A_{11} - a & A_{12} & A_{13} \\ A_{21} & A_{22} - a & A_{23} \\ A_{31} & A_{32} & A_{33} - a \end{vmatrix} = 0. \tag{13}$$

the result is a cubic polynomial equation for a, from which three eigenvalues can be extracted. If A is self-adjoint, we already know that these solutions, which are the eigenvalues, are real. Once the three values of a are found, the corresponding ψ_i can be deduced for each value.