Quantum Mechanics: Matrix formulation

Operators as matrices

In quantum mechanics one often deals with systems which have a discrete, finite dimensional Hilbert space. In such situations, sometimes it is covenient to use a different kind of formulation of quantum mechanics. Let use consider an operator $\hat{A}$ and an arbitrary complete set of eigenstates $\{|p_i\rangle\}$. The operator $\hat{A}$ can be represented in this basis by simply multiplying with a unit operator (denonted by a complete set) on either side of it:

$$\begin{aligned}\hat{A} &= \sum_{m=1}^{N} |p_m\rangle\langle p_m|\hat{A}\sum_{n=1}^{N}|p_n\rangle\langle p_n| \\ &= \sum_{m,n}\langle p_m|\hat{A}|p_n\rangle|p_m\rangle\langle p_n| \\ &= \sum_{m,n} A_{mn}|p_m\rangle\langle p_n|, \end{aligned} \tag{1}$$

where $A_{mn} = \langle p_m|\hat{A}|p_n\rangle$. Since the size of the Hilbert space is N, there are N^2 number of terms A_{mn}. It looks obvious that these elements can be written as a matrix

$$A = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1N} \\ A_{21} & A_{22} & \dots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \dots & A_{NN} \end{pmatrix}$$

States as matrices

We already know that a state can be written in terms of basis states

$$|\psi\rangle = \sum_{n=1}^{N}\langle p_n|\psi\rangle|p_n\rangle.$$

The elements $\langle p_n|\psi\rangle$ are N in number. The operator $\hat{A}$ acting on the state $|\psi\rangle$ can be written as

$$\begin{aligned}\hat{A}|\psi\rangle &= \sum_{m,n} A_{mn}|p_m\rangle\langle p_n|\sum_{k=1}^{N}\langle p_k|\psi\rangle|p_k\rangle \\ &= \sum_{m,n} A_{mn}\langle p_n|\psi\rangle|p_m\rangle. \end{aligned} \tag{2}$$

This does look like a square matrix multiplied with a column matrix. This suggests that the ket state can be written as a column matrix:

$$|\psi\rangle = \begin{pmatrix} \langle p_1|\psi\rangle \\ \langle p_2|\psi\rangle \\ \vdots \\ \langle p_N|\psi\rangle \end{pmatrix}$$

It is but natural to expect that the bra state will be represented by a row matrix, but with a complex conjugate:

$$\langle\psi| = \begin{pmatrix}\langle\psi|p_1\rangle & \langle\psi|p_2\rangle & \dots & \langle\psi|p_N\rangle\end{pmatrix}.$$

The inner product of two states is a number:

$$\langle\phi|\psi\rangle = \begin{pmatrix}\langle\phi|p_1\rangle & \langle\phi|p_2\rangle & \dots & \langle\phi|p_N\rangle\end{pmatrix}\begin{pmatrix}\langle p_1|\psi\rangle \\ \langle p_2|\psi\rangle \\ \vdots \\ \langle p_N|\psi\rangle\end{pmatrix}$$

It can be verified that the above yields just the normal inner product of quantum mechanics

$$\langle\phi|\psi\rangle = \langle\phi|\sum_{n=1}^{N}|p_n\rangle\langle p_n||\psi\rangle = \sum_{n=1}^{N}\langle\phi|p_n\rangle\langle p_n|\psi\rangle.$$

From the above analysis it is clear that quantum mechanics in finite dimensional Hilbert space can be done by representing operators and states as matrices. However, one has to choose a basis for doing so. The matrix for an operator will look different in different bases.

Diagonal representation

Let us choose the eigenstates of the operator $\hat{A}$ as our basis:

$$\hat{A}|a_n\rangle = \alpha_n|a_n\rangle,$$

where α_n are the eigenvalues of $\hat{A}$. The *matrix elements* of $\hat{A}$ will now look like:

$$A_{mn} = \langle a_m|\hat{A}|a_n\rangle = \alpha_n\delta_{mn}.$$

This means that the matrix for $\hat{A}$ is now is a diagonal matrix with the eigenvalues as the diagonal elements

$$A = \begin{pmatrix}\alpha_1 & 0 & \dots & 0 \\ 0 & \alpha_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \alpha_N\end{pmatrix}.$$

An eigenstate of $\hat{A}$, (say) $|a_2\rangle$ will be a column matrix, with the elements given by $\langle a_n|a_2\rangle$. Clearly the 2nd element will be 1, and the rest will be zero:

$$|a_2\rangle = \begin{pmatrix}0 \\ 1 \\ 0 \\ \vdots \\ 0\end{pmatrix}$$

We started by solving the problem of a paricle in a box, by writing the time-independent Schrödinger equation

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$$

as a differential equation. In terms of matrices, solving the time-independent Schrödinger equation of another system would amount to finding a basis in which the matrix for $\hat{H}$ is diagonal. The diagonal elements of the matrix will be the energy eigenvalues. The way one would proceed is by choosing a basis one is familiar with, and then writing $\hat{H}$ as a matrix in that basis. Once H_{mn} is generated, it can be treated like any other matrix, and diagonalized using standard methods. The eigenvalues thus obtained will be the values of energy of the system. In situations where a problem cannot be solved analytically, one may look for numerical solution using a computer. The advantage in using a computer is that one can deal system with large Hilbert space, which produce a large-dimensional matrix for the Hamiltonian. The large matrix can be diagonalized using state of the art numerical techniques. This is the approach in solving many problems in condensed matter physics.

Adjoint of an operator

We know that the adjoint of an operator is given by

$$\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*,$$

for any $|\psi\rangle, |\phi\rangle$. We choose a basis $\{|p_n\rangle\}$, and write the adjoint relation for two states of this basis, and find

$$\begin{aligned}\langle p_n|\hat{A}^\dagger|p_m\rangle &= \langle p_m|\hat{A}|p_n\rangle^* \\ A^\dagger_{nm} &= A^*_{mn}\end{aligned} \tag{3}$$

holds for all m, n. However, $A^\dagger_{nm}$ and A_{mn} are elements of the matrices for the operators $\hat{A}^\dagger$ and $\hat{A}$, respectively. Then eqn. (**??**) implies that the matrix for $\hat{A}^\dagger$ is obtained by taking a transpose of the matrix for $\hat{A}$, and taking complex conjugate of the elements. That is also the stanndard definition of the Hermitian adjoint of a matrix.

Matrix formulation of quantum mechanicsis particularly useful in dealing with the problems related to angular momenta, as the Hilbert space is finite there.