Matrix Mechanics

PHYS 2210 - Class 22

Why Matrix Mechanics?

- It is possible to represent the expansion of a quantum state as a vector with the expansion coefficients.
- Operators can be represented as matrices.
- Once we have represented states and operators correctly, the rules of matrix mathematics and linear algebra can be used to set up calculations.

A matrix representation of expansions

This will provide a compact way of describing eigenvalue expansions.

First let's consider expressing an ordinary two dimensional vector in Cartesian coordinates.

$$\vec{r} = r_x \hat{\imath} + r_y \hat{\jmath}$$

By convention we can represent this as a column vector with the coefficients for each unit vector:

$$\vec{r} = \begin{pmatrix} r_x \\ r_y \end{pmatrix}$$

Eigenfunction expansions

Assume the operator A_{op} has two orthonormal eigenfunctions, $\psi_1(x)\ and\ \psi_2(x)$ with eigenvalues $a_1 and\ a_2$.

An arbitrary state of the particle is given by: $\psi(x) = c_1\psi_1 + c_2\psi_2$.

Similarly to spatial vectors we can express $\psi(x)$ as a vector of components.

$$\psi(x) = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

So that $\psi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\psi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

In bra-ket notation: $|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ is a column vector.

Eigenfunction expansions

$\langle\psi| = \psi^* = (c_1^* \; c_2^*)$ is a row vector, so that the inner product yields the probability density:

$$\langle\psi|\psi\rangle = c_1^* c_1 + c_2^* c_2$$

We can extend this to calculate the inner product (overlap integral) of two arbitrary states:

$\psi = c_1\Psi_1 + c_2\psi_2 = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ and

$\phi = d_1\psi_1 + d_2\psi_2 = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}$

So $\langle\psi|\phi\rangle = c_1^* d_1 + c_2^* d_2 = (c_1^* \;\; c_2^*)\begin{pmatrix} d_1 \\ d_2 \end{pmatrix}$

Matrix representation of an operator

How do we represent A_{op} in $|\psi'\rangle = A_{op}|\psi\rangle$?

Where $|\psi\rangle = \Sigma_i c_i \ |u_i\rangle \ and \ |\psi'\rangle = \Sigma_i c_i'|u_i\rangle$

where $c_i' = \langle u_i|\psi'\rangle = \langle u_i|A_{op}|\psi\rangle$

and so

$$\begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \dots & \dots & \dots \end{pmatrix} \text{ where } A_{ij} = \langle u_i|A_{op}|u_j\rangle$$

Matrix expression or an operator - by example

The operator A_{op} thus does the following to the wavefunction:

$$A_{op}\psi = c_1 a_1 \psi_1 + c_2 a_2 \psi_2$$

or $A_{op}\psi = A_{op}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} a_1 & 0 \\ 0 & a_2 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

The fact that the A_{op} matrix is diagonal actually tells us that $\psi_1 and\ \psi_2$ are eigenfunctions of A_{op}.

As an example of using matrix representations:

Let's define the operator B_{op} according to:

$B_{op} \equiv c_2\psi_1 + c_1\psi_2$ (note the switcheroo)

In vector form: $B_{op}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} c_2 \\ c_1 \end{pmatrix}$

The B matrix that does this is: $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} c_2 \\ c_1 \end{pmatrix}$$

So we see that B_{op} and A_{op} do not share any eigenfunctions, because the B matrix has no diagonal components..

Let's now try to find the eigenvalues of $B_{op}\psi = b\psi$.

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = b\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} bc_1 \\ bc_2 \end{pmatrix} = \begin{pmatrix} b & 0 \\ 0 & b \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Or $\begin{pmatrix} -b & 1 \\ 1 & -b \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$=0

You might recognize problems of this type from linear algebra.

In order for there to be a non-trivial solution, we must have: $\begin{vmatrix} -b & 1 \\ 1 & -b \end{vmatrix} = 0$ and thus $b^2 = 1 \; or \; b = \pm 1$

For $b = 1$, we have $\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$=0

or $c_1 = c_2$ and the eigenfunction of B_{op} expressed in terms of eigenfunctions of A_{op} is $\psi_{B1} = c_1\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and if we normalize it:

$$\psi_{B1}(norm\, eigen) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

For $b = -1$, we have $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$=0

or $c_1 = -c_2$ and the eigenfunction of B_{op} expressed in terms of eigenfunctions of A_{op} is $\psi_{B-1} = c_1\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

and if we normalize it:

$$\psi_{B-1}(norm\ eigen) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

This was complicated way to solve a simple problem, but it displays the way in which matrix approaches can be used.

Spin

- Assume the eigenfunctions of the z-component of the spin of a spin ½ particle are χ_+ for a spin aligned along a magnetic field and χ_- for an anti-aligned spin, so that:
  $S_z\chi_+ = \frac{\hbar}{2}\chi_+$ and $S_z\chi_- = -\frac{\hbar}{2}\chi_-$
- An arbitrary state can be represented by a vector of the coefficients:

$$\chi_{arb} = \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \; and \; \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Spin Matrices

Representing the eigenfunctions as vectors:

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \ and \ \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We can find the matrix operator by assuming

$$S_z = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

And we want $S_z \chi_+ = \frac{\hbar}{2} \chi_+$ or $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ c \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

So that $a = 1 \ and \ c = 0$.

We also want $S_{zop} \chi_- = \frac{\hbar}{2} \begin{pmatrix} 1 & b \\ 0 & d \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

So that $b = 0 \ and \ d = -1$

The operator for the z-component of the spin angular momentum can therefore be represented as:

$$S_{zop} = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Spin Matrices 2

Let's find the matrix for S_{op}^2.

We know that a particle in a spin up state satisfies:

$$S_{op}^2\chi_+ = \big(s(s+1)\big)\hbar^2\chi_+ = \frac{3}{4}\hbar^2\chi_+$$

$$S_{op}^2\chi_- = \big(s(s+1)\big)\hbar^2\chi_- = \frac{3}{4}\hbar^2\chi_-$$

To find the eigenfunctions and values we write S^2 as a matrix with unknown elements:

$$S_{op}^2 = \begin{pmatrix} e & f \\ g & h \end{pmatrix}$$

So that $S_{op}^2\chi_+ = \begin{pmatrix} e & f \\ g & h \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} e \\ g \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

And thus $\begin{pmatrix} e \\ g \end{pmatrix} = \begin{pmatrix} \frac{3}{4}\hbar^2 \\ 0 \end{pmatrix}$. Similarly, $f = 0\ and\ g = \frac{3}{4}\hbar^2$

Spin 3

Putting the coefficients into the matrix representation:

$$S_{op}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

We can also deduce the operators for S_x and S_y.

$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

and using a standard notation:$S_x = \frac{\hbar}{2}\sigma_x$

Where $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$…

The sigma’s are called the Pauli spin matrices.

Spin Matrices

- Note that the matrices for $S_z \ and \ S^2$ are diagonal, indicating that $\chi_+ \ and \ \chi_-$ are eigenfunctions of these operators.
- The matrices for $S_x \ and \ S_y$ are not diagonal, indicating that $\chi_+ \ and \ \chi_-$ are not eigenfunctions of these operators.

Some Matrix Math

- We can now find the commutator of $S_x and\ S_y$.
  $[S_x, S_y]$
  $= \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
  $= \frac{\hbar^2}{4}\left(\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}\right) = \frac{\hbar^2}{2}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$

so $[S_x, S_y] = i\hbar S_z$