Eigenvalues and Eigenvectors

There may be a set of vectors in $\mathbb{V}$ where the operator $\hat{A}$ only changes the vectors length

$$\hat{A}|a\rangle = \lambda|a\rangle$$

$|a\rangle$ is an <u>eigenvector</u> of $\hat{A}$ and λ is its eigenvalue.

We will label the eigenvectors of $\hat{A}$ with their eigenvalues,

$$\hat{A}|a_i\rangle = a_i|a_i\rangle$$

Properties of Hermitian Operators

I. The eigenvalues are real.

II. Eigenvectors with different eigenvalues are orthogonal

$$\text{If } a_i \neq a_j \Rightarrow \langle a_j|a_i\rangle = 0$$

III Eigenvectors span the space

<u>Observable</u> – A Hermitian operator s.t. its eigenvecters span $\mathbb{V}$.

$\Rightarrow$ All measurable physical quantities are represented by observables.

$\Rightarrow$ Why? Measurable quantities are real and something must be measured in each experiment.

Calculating Eigenvalues

Sometimes, but not often, we can calculate the eigenvalues of an operator directly from its general definition.

For example, consider the projection operator

$$\hat{P} = \sum_i |a_i\rangle\langle a_i|$$

that projects $|a\rangle$ onto a subspace spanned by $\{|a_i\rangle\}$.

If $|p\rangle$ is an eigenvector and λ the eigenvalue

$$\hat{P}|p\rangle = \lambda|p\rangle$$

If we project again, we must also have

an $$\hat{P}^2|p\rangle = \lambda|p\rangle = \lambda^2|p\rangle$$

$$\Longrightarrow \lambda = 0, 1$$

In most circumstances, we will have to find the eigenvalues and vectors by writing the operator and vectors in component form in some basis.

Ex The likely place to start is the free particle. Its total energy is $H = \frac{P^2}{2m}$ so to find the allowed energies we let $P \to \hat{P}$

$$H \to \hat{H} = \frac{\hat{P}^2}{2m}$$ and we solve the

eigenvalue problem

$$\hat{H}|a\rangle = E|a\rangle$$

unfortunately E is continuous and the basis we need to use is also continuous. Try something harder that ends up simpler.

Ex Simple Harmonic Oscillator

Total Energy $H = \frac{P^2}{2m} + \frac{1}{2} k x^2$

Operator $\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} k \hat{X}^2$

Eigenvalue Problem

$$\hat{H} |a\rangle = E |a\rangle$$

to find energies.

Still too hard, E discrete but but an infinite number of values allowed $\Rightarrow$ basis countable but infinite.

Ex Consider a charged particle with angular momentum $\sqrt{2}\hbar$ in a magnetic field $\vec{B} = B_0 \hat{z}$.

The total energy is $H = -\vec{\mu} \cdot \vec{B}$ where $\vec{\mu}$ is the magnetic moment.

$$H = -\gamma \vec{L} \cdot \vec{B}$$

where $\vec{L}$ is the angular momentum and γ is called the gyromagnetic ratio, For orbital angular momentum, $\gamma = \frac{q}{2m}$.

The Hamiltonian operator for this system will turn out to be

$$\hat{H} = -\frac{\gamma B_0 \hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

~~So how do we~~

Eigenvalue problem becomes a matrix problem

$$\hat{H}|a\rangle = E|a\rangle$$

$$\Longrightarrow \quad -\frac{\gamma B_0 \hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = E \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

Find E, a_i

How do we get from abstract vector spaces to a normal matrix problem? $\Rightarrow$ closure.

The Hamiltonian operator is an observable and is therefore Hermitian ($\hat{H}^\dagger = \hat{H}$) and its eigenvectors span the space. For angular momentum systems, it is traditional to use the eigenvectors of the z-component of angular momentum as basis vectors. The z-component has 3 eigenvectors, $|\hbar\rangle$, $|0\hbar\rangle$, $|-\hbar\rangle$. If we use this order, $|a_1\rangle = |\hbar\rangle$, $|a_2\rangle = |0\hbar\rangle$, $|a_3\rangle = |-\hbar\rangle$ we can write any vector uniquely as $|\psi\rangle = c_1|a_1\rangle + c_2|a_2\rangle + c_3|a_3\rangle$ and represent $|\psi\rangle$ by the 3-tuple (c_1, c_2, c_3).

The vectors $\{|a_i\rangle\}$ are orthonormal so

$$\langle a_i | a_j \rangle = \delta_{ij}$$

Therefore to find c_1 we can use

$$c_1 = \langle a_1 | \psi \rangle = c_1 \overset{1}{\langle a_1 | a_1 \rangle} + c_2 \overset{0}{\langle a_1 | a_2 \rangle}$$
$$+ c_3 \underset{0}{\langle a_1 | a_3 \rangle}$$

We will represent kets as column vectors

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} \langle a_1 | \psi \rangle \\ \langle a_2 | \psi \rangle \\ \langle a_3 | \psi \rangle \end{pmatrix}$$

Our eigenvalue problem is

$$\hat{H} |\psi\rangle = E |\psi\rangle$$

The ith component of this expression is

$$\langle a_i | \hat{H} | \psi \rangle = E \langle a_i | \psi \rangle = c_i E$$

<u>Use closure</u>

$$\hat{1} = \sum |a_j\rangle \langle a_j|$$

$$\langle a_i | \hat{H} \hat{1} | \psi \rangle = \sum_j \langle a_i | \hat{H} | a_j \rangle \langle a_j | \psi \rangle$$

$$\langle a_i | \hat{H} | \Psi \rangle = \sum_j H_{ij} c_j = E c_i$$

where $H_{ij} \equiv \langle a_i | \hat{H} | a_j \rangle$

This looks completely like matrix multiplication with the matrix representing $\hat{H}$ as

$$\begin{pmatrix} \langle a_1 | \hat{H} | a_1 \rangle & \langle a_1 | \hat{H} | a_2 \rangle & \langle a_1 | \hat{H} | a_3 \rangle \\ \langle a_2 | \hat{H} | a_1 \rangle & \langle a_2 | \hat{H} | a_2 \rangle & \langle a_2 | \hat{H} | a_3 \rangle \\ \langle a_3 | \hat{H} | a_1 \rangle & \langle a_3 | \hat{H} | a_2 \rangle & \langle a_3 | \hat{H} | a_3 \rangle \end{pmatrix}$$

and we can do this with an operator.

This is the representation of $\hat{H}$ in the $\{|a_i\rangle\}$ basis.

Our eigenvalue problem becomes

$$\begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

For our spin system,

$$-\frac{\gamma B_0 \hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

Define $E' = -\dfrac{\sqrt{2}\, E}{\gamma B_0 \hbar}$

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = E' \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

This is a standard eigenvalue problem and has a standard method of solution. Suppose we have a matrix $\overleftrightarrow{T}$ and the identity matrix $\overleftrightarrow{1}$

We want to multiply $\overleftrightarrow{T}$ by the vector $\vec{c}$ and get the same vector back, possibly rescaled.

$$\overleftrightarrow{T}\,\vec{c} = \lambda \vec{c}$$

Matrix $\overleftrightarrow{T}$

Vector represented as column $\vec{c}$.

where λ is an eigenvalue.

$\Longrightarrow$ Insert the identity matrix

$$\overleftrightarrow{1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\overleftrightarrow{T}\,\vec{c} = \lambda \overleftrightarrow{1}\,\vec{c} \quad \text{or} \quad \left(\overleftrightarrow{T} - \lambda \overleftrightarrow{1}\right)\vec{c} = 0$$

$\Longrightarrow$ The condition for the second expression to be solvable is

$$\det\left(\overleftrightarrow{T} - \lambda\overleftrightarrow{1}\right) = 0$$

$$\det\begin{pmatrix} T_{11}-\lambda & T_{12} & T_{13} \\ T_{21} & T_{22}-\lambda & T_{23} \\ T_{31} & T_{32} & T_{33}-\lambda \end{pmatrix} = 0$$

$\Rightarrow$ This condition gives a polynomial in λ called the characteristic equation. The solutions to the characteristic equation are the eigenvalues.

Lets try Let $E' = \lambda$

$$\det(\overleftrightarrow{H} - \lambda \overleftrightarrow{1}) = 0$$

$$\det\begin{pmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 1 \\ 0 & 1 & -\lambda \end{pmatrix} = 0$$

$$-\lambda(\lambda^2-1) \quad -1(-\lambda) = 0$$

$$-\lambda(\lambda^2-2) = 0$$

Eigenvalues $\lambda = 0, \pm\sqrt{2}$

Eigenvectors

$\lambda = 0$ — Plug into $\overleftrightarrow{T} - (\lambda=0)\overleftrightarrow{I} = 0$

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0$$

First row $\quad a_2 = 0$

Second row $\quad a_1 + a_3 = 0 \qquad$ Pick $a_1 = 1$

$\Rightarrow a_3 = -1$

$$|\lambda=0\rangle = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

Normalize

$$|\lambda=0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

Eigenvector $\lambda = +\sqrt{2}$

$$\begin{pmatrix} -\sqrt{2} & 1 & 0 \\ 1 & -\sqrt{2} & 1 \\ 0 & 1 & -\sqrt{2} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0$$

First Row $\quad -\sqrt{2}\, a_1 + a_2 = 0$

Second Row $\quad a_1 - \sqrt{2}\, a_2 + a_3 = 0$

Select $a_1 = 1, \Rightarrow a_2 = \sqrt{2}$ First row

Second Row $\quad 1 - \sqrt{2}\sqrt{2} + a_3 = 0$

$$-1 + a_3 = 0$$

$$a_3 = 1$$

$$|\lambda = \sqrt{2}\rangle = \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$$

Normalize $\quad |\lambda = \sqrt{2}\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$

Eigenvector $\lambda = -\sqrt{2}$

$$\begin{pmatrix} \sqrt{2} & 1 & 0 \\ 1 & \sqrt{2} & 1 \\ 0 & 1 & \sqrt{2} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0$$

First Row

$$\sqrt{2}\, a_1 + a_2 = 0$$

If $a_1 = 1$, $a_2 = -\sqrt{2}$

Second Row

$$a_1 + \sqrt{2}\, a_2 + a_3 = 0$$

$$1 - \sqrt{2}\,\sqrt{2} + a_3 = 0$$

$$a_3 = 1$$

$$|\lambda = -\sqrt{2}\rangle = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

Normalize

$$|\lambda = -\sqrt{2}\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

Some matrix stuff

What does the adjoint look like in matrix land?

If $$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}$$

$$\hat{A}^{+} = \left(\hat{A}^{T}\right)^{*}$$ complex conjugate

Dfn Transpose ($\hat{A}^T$) Reflect $\hat{A}$ about diagonal

$$A_{ij} \rightarrow A_{ji}$$

$$\hat{A}^{+} = \begin{pmatrix} A_{11}^{*} & A_{21}^{*} & A_{31}^{*} \\ A_{12}^{*} & A_{22}^{*} & A_{32}^{*} \\ A_{13}^{*} & A_{23}^{*} & A_{33}^{*} \end{pmatrix}$$

So what is $\langle a|$?

$$\langle a| \neq |a\rangle^{+}$$

If

$$|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$\langle a| = |a\rangle^{+} = \begin{pmatrix} a_1^* & a_2^* & a_3^* \end{pmatrix}$$

<u>Check Orthonormal</u>

$$\langle \lambda = 1 | \lambda = \sqrt{2} \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$$

$$= 0 \checkmark$$

~~orth~~ Other vectors likewise orthogonal.

Wolfram Alpha computational knowledge engine

eigenvectors {{0,1,0},{1,0,1}, {0,1,0}}

Input:

$$\text{Eigenvectors}\left[\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\right]$$

Result:

$v_1 \approx \{1, -1.41421, 1\}$

$v_2 \approx \{1, 1.41421, 1\}$

$v_3 \approx \{-1, 0, 1\}$

Corresponding eigenvalues:

$\lambda_1 = -\sqrt{2}$

$\lambda_2 = \sqrt{2}$

$\lambda_3 = 0$