## Lecture 5

## Vector Spaces and Linear Algebra:

Vector Representation of Wave States in Hilbert Spaces

## Reading:

Notes and Brennan Chapter 1.6-1.7

## Fundamental Expansion Postulate

Basis vectors (a minimal set of orthogonal vectors that uniquely and completely describes all of vector space) can be added together to construct any point in the vector space.

Example: the unit vectors in Cartesian coordinates.

Similarly, we can think of orthogonal sets of wave functions as vectors and treat them similarly to simple vectors - i.e. add linear combinations of basis wave function sets to result in any arbitrary wave function within the wave space.

Lee Algebra is often used here: Lee was a pure mathematician who described his Linear Algebra as "finally a mathematical formulation that the physicists cannot corrupt with a useful purpose [paraphrase - not direct quote]".

## Fundamental Expansion Postulate

Consider the case of two orthogonal wave functions (two states):
If $\Psi_{\mathrm{n}}$ and $\Psi_{\mathrm{m}}$ are orthogonal, then

$$
\int_{-\infty}^{\infty} \Psi_{m}^{*} \Psi_{n} d v=\delta_{m n}
$$

However, in general, if $\Psi_{n}$ and $\Psi_{\mathrm{m}}$ are orthogonal, then nothing can be said about


$$
\int_{-\infty}^{\infty} \Psi_{m}^{*} \xi_{o p} \Psi_{n} d v^{?}=K \delta_{m n}
$$

because $\xi_{\text {op }}$ may rotate $\Psi_{\mathrm{n}}$ into a projection of $\Psi_{m}$. However, if $\Psi_{n}$ is an Eigenfunction of $\xi_{\text {op }}$ then

$$
\int_{-\infty}^{\infty} \Psi_{M}^{*} \xi_{o p} \Psi_{n} d v=\lambda_{n} \int_{-\infty}^{\infty} \Psi_{M}^{*} \Psi_{n} d v=\lambda_{n} \delta_{m n}
$$

## Fundamental Expansion Postulate

A basis set is a minimum set of functions that completely spans the space (i.e. all regions in space can be derived from linear combinations of the basis set).

Example: Fourier Series or unit vectors $\mathbf{x}, \mathbf{y}$, z.
Since Eigenfunctions of a Hermitian operator having unequal Eigenvalues are mutually orthogonal if they are complete, they must form a basis set.

The Fundamental Expansion Postulate states that every physical observable can be represented by a Hermitian operator with a complete basis set of Eigenfunctions, $\Psi_{1}, \Psi_{2}, \Psi_{3}, \ldots, \Psi_{n}$ and every physical state $\Psi$ can be expanded as a linear combination of Eigenstates as

$$
\Psi=\sum_{i} c_{i} \Psi_{i}
$$

Where each coefficient is given as:

$$
c_{i}=\int \Psi_{i}^{*} \Psi d v
$$

This is sort of like a dot-product operation with a unit vector in normal vector Linear algebra: For example: if you want to know the $y^{\text {th }}$ coefficient of the vector $\mathbf{r}=2 \mathbf{x}+3 \mathbf{y}+7 \mathbf{z}$, where $\mathbf{x}, \mathbf{y}$, and $\mathbf{z}$ are unit vectors (basis vectors) simply take $\mathbf{r}^{\circ} \mathbf{y}$

## Fundamental Expansion Postulate

Proof:
Let $\mathrm{A}_{\mathrm{op}}$ be a Hermitian operator with Eigenfunctions, $\Psi_{1}, \Psi_{2}, \Psi_{3}, \ldots, \Psi_{\mathrm{n}}$ and Eigenvalues $\mathbf{A}_{1}, \mathbf{A}_{2}, \mathbf{A}_{3}, \ldots \mathbf{A}_{\mathrm{n}}$. The arbitrary physical state $\Psi$ can be expanded as a linear combination of Eigenstates as,

$$
\Psi=\sum_{i} c_{i} \Psi_{i}
$$

And the expectation value, $<\mathrm{A}>$ is then given by,

$$
\langle A\rangle=\int \Psi^{*} A_{o p} \Psi d v
$$

Therefore...

## Fundamental Expansion Postulate

## Proof (cont'd):

$$
\begin{aligned}
& \langle\mathrm{A}\rangle=\int \Psi^{*} \mathrm{~A}_{\mathrm{op}} \Psi \mathrm{dv} \\
& \langle\mathrm{~A}\rangle=\int\left(\sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}}{ }^{*} \Psi_{\mathrm{i}}{ }^{*}\right) \mathrm{A}_{\mathrm{op}}\left(\sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}\right) \mathrm{dv} \\
& \langle\mathrm{~A}\rangle=\int\left(\mathrm{c}_{1}{ }^{*} \Psi_{1}{ }^{*}+\mathrm{c}_{2}{ }^{*} \Psi_{2}{ }^{*}+\ldots \quad \mathrm{c}_{\mathrm{n}}{ }^{*} \Psi_{\mathrm{n}}{ }^{*}\right) \mathrm{A}_{\mathrm{op}}\left(\mathrm{c}_{1} \Psi_{1}+\mathrm{c}_{2} \Psi_{2}+\ldots \quad \mathrm{c}_{\mathrm{n}} \Psi_{\mathrm{n}}\right) \mathrm{dv} \\
\begin{array}{c}
\text { Now using the } \\
\text { Eigenvalue } \\
\text { relationship }
\end{array} \longrightarrow & \langle\mathrm{A}\rangle=\int\left(\mathrm{c}_{1}{ }^{*} \Psi_{1}{ }^{*}+\mathrm{c}_{2}{ }^{*} \Psi_{2}{ }^{*}+\ldots \quad \mathrm{c}_{\mathrm{n}}{ }^{*} \Psi_{\mathrm{n}}{ }^{*}\right)\left(\mathrm{c}_{1} \mathrm{~A}_{1} \Psi_{1}+\mathrm{c}_{2} \mathrm{~A}_{2} \Psi_{2}+\ldots \quad \mathrm{c}_{\mathrm{n}} \mathrm{~A}_{\mathrm{n}} \Psi_{\mathrm{t}}\right. \\
& \text { but the } \mathrm{c}_{\mathrm{i}} \text { s are just numbers and since } \\
& \int \Psi_{\mathrm{i}}{ }^{*} \Psi_{\mathrm{j}} \mathrm{dv}=\delta_{\mathrm{ij}} \\
& \text { all " cross terms cancel", leading to } \\
& \langle\mathrm{A}\rangle=\sum_{\mathrm{i}}\left(\mathrm{~A}_{\mathrm{i}}\left|\mathrm{c}_{\mathrm{i}}\right|^{2} \int \Psi_{\mathrm{i}}{ }^{*} \Psi_{\mathrm{i}} \mathrm{dv}\right) \\
& \text { and since } \Psi \text { is normalized, } \\
& \langle\mathrm{A}\rangle=\sum_{\mathrm{i}} \mathrm{~A}_{\mathrm{i}}\left|\mathrm{c}_{\mathrm{i}}\right|^{2} \\
& \text { Thus, }\langle\mathrm{A}\rangle \text { is a weighted average of the } \\
& \text { Eigenvalues, } \mathrm{A}_{\mathrm{i}} \text { where the weights are the }\left|\mathrm{c}_{\mathrm{i}}\right|^{2}{ }^{\prime} \mathrm{s}
\end{aligned}
$$

## Fundamental Expansion Postulate

Proof (cont'd):
But how do we find the $\left|\mathbf{c}_{\mathrm{j}}\right|^{\mathbf{2}} \mathbf{~} \mathbf{s}$ ? Given:

$$
\Psi=\sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}
$$

Multiply by $\Psi_{j}{ }^{*} \longrightarrow \Psi_{j}{ }^{*} \Psi=\sum_{i} \mathrm{c}_{\mathrm{i}} \Psi_{j}{ }^{*} \Psi_{\mathrm{i}}$
$\underset{\substack{\text { Integrate over all } \\ \text { space }}}{ } \int \Psi_{\mathrm{j}}{ }^{*} \Psi \mathrm{dv} v=\int\left(\sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{j}}{ }^{*} \Psi_{\mathrm{i}}\right) \mathrm{dv}$

$$
\begin{aligned}
& \int \Psi_{j}^{*} \Psi d v=\sum_{i} c_{i} \delta_{i j} \\
& \int \Psi_{j}^{*} \Psi d v=c_{i}
\end{aligned}
$$

Before a measurement, the particle can be in an unidentifiable state $\Psi$ (but is made up of a linear combination of Eigenstates). However, once measured, the particle is in a known Eigenstate, $\Psi_{i}$, with known measurable variable $\mathbf{A}_{i}$. The term "collapsing into known state $\Psi_{i}$ " is often used. The $\left|c_{i}\right|^{2}$ ' $s$ are the probability of collapse (probability that a measurement corresponding to Hermitian operator $\mathbf{A}_{\text {op }}$ of the particle in arbitrary state $\Psi$ will result in an observable $\mathbf{A}_{\mathbf{i}}$ ).

Hilbert Space: Linear Vector Spaces using "Vector Functions" Since we can treat orthogonal wave functions as vectors, we can define many linear algebra functions that apply to wave functions as well.

Distribitive Addition: $\Psi_{m}+\Psi_{n}=\Psi_{n}+\Psi_{m}$ and $\Psi_{m}+\left(\Psi_{n}+\Psi_{1}\right)=\left(\Psi_{n}+\Psi_{m}\right)+\Psi_{1}$
Scalor Multiplication: $\mu\left(\lambda \Psi_{\mathrm{m}}\right)=(\mu \lambda) \Psi_{\mathrm{m}}$ and $\lambda\left(\Psi_{\mathrm{m}}+\Psi_{\mathrm{n}}\right)=\lambda \Psi_{\mathrm{m}}+\lambda \Psi_{\mathrm{n}}$
Existance of a Null State: $\Psi_{\mathrm{m}}+\Psi_{\mathrm{o}}=\Psi_{\mathrm{m}}$
Linear Indepencence of all States: If all $\lambda_{i} \neq 0$ then $\sum_{i} \lambda_{i} \Psi_{i} \neq 0$ for all $i$

## Linear Vector Spaces

State projections onto each other:
While basis vectors are orthogonal, any two generalized states (each made up of linear combinations of basis states) may not be. Thus, we can define an "overlap operation" similar to a dot product in traditional linear algebra. Similarly to the dot product, this operation returns a scalar representing how much overlap is between the two states:

$$
\begin{gathered}
d=\int_{-\infty}^{\infty} \Psi_{m}^{*} \Psi_{\mathrm{n}} \mathrm{dv} \\
\mathrm{~d}=\int_{-\infty}^{\infty}\left(\Psi_{\mathrm{m}}^{*}\right)\left(\Psi_{\mathrm{n}}\right) \mathrm{dv} \\
\mathrm{~d}=\int_{-\infty}^{\infty}\left(\sum_{\mathrm{i}} \mathrm{a}_{\mathrm{i}}^{*} \Psi_{\mathrm{i}}^{*}\right)\left(\sum_{\mathrm{j}} \mathrm{~b}_{\mathrm{j}} \Psi_{\mathrm{j}}\right) \mathrm{dv} \\
\mathrm{~d}=\sum_{\mathrm{i}} \sum_{\mathrm{j}} \mathrm{a}_{\mathrm{i}} \mathrm{~b}_{\mathrm{j}}^{*} \int_{-\infty}^{\infty} \Psi_{\mathrm{i}}^{*} \Psi_{\mathrm{j}} \mathrm{dv}
\end{gathered}
$$

but again if we used orthogonal basis functions, $\Psi_{i}$ and $\Psi_{j}$,

$$
\begin{gathered}
\mathrm{d}=\sum_{\mathrm{i}} \sum_{\mathrm{j}} \mathrm{a}_{\mathrm{i}}^{*} \mathrm{~b}_{\mathrm{j}} \delta_{i j} \\
\mathrm{~d}=\sum_{\mathrm{i}} \mathrm{a}_{\mathrm{i}}^{*} \mathrm{~b}_{\mathrm{i}}
\end{gathered}
$$

## Linear Vector Spaces

What is an Operator in the Wave space formulism?
An operator merely maps one wave state to another with both initial and final states being in the Hilbert space and thus, both initial and final states can be represented by linear combinations of the basis vector states. Formally this is simply:

$$
\Psi_{\mathrm{new}}=\xi_{\mathrm{op}} \Psi_{\mathrm{old}}
$$

Thus an operator merely changes the state from one state to another. Consider the simple " 5 times" operator: The new state is mathematically different for the old state by a factor of 5 .

## Matrix Methods in Quantum Mechanics

The Fundamental Expansion Postulate can be rewritten in matrix form. Every physical observable can be represented by a Hermitian operator with a complete basis set of Eigenfunctions, $\Psi_{1}, \Psi_{2}, \Psi_{3}, \ldots, \Psi_{n}$ and every physical state $\Psi$ can be expanded as a linear combination of Eigenstates as

$$
\begin{aligned}
& \Psi=\sum_{i} c_{i} \Psi_{i} \\
& \Psi=\left[\begin{array}{lllll}
c_{1} & c_{2} & c_{3} & \cdots & c_{n}
\end{array}\right]\left[\begin{array}{c}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3} \\
\vdots \\
\Psi_{n}
\end{array}\right] \\
& c_{i}=\int \Psi_{i}^{*} \Psi d v
\end{aligned}
$$

Integrals like these that we have been using all semester are often called matrix elements - now you can see why.

## Matrix Methods in Quantum Mechanics

Thus, every generalized state can be represented by a vector, $c$, which are the coefficients of the basis wave states (coefficients of the basis vectors).

Since an operator merely changes from one state to another, the operator then can be represented as a matrix as well. Consider:

$$
\begin{gathered}
\Psi_{c}=\sum_{i} c_{i} \Psi_{i} \text { and } \Psi_{a}=\sum_{i} a_{i} \Psi_{i} \\
\Psi_{c}=\left[\begin{array}{lllll}
c_{1} & c_{2} & c_{3} & \cdots & c_{n}
\end{array}\right]\left[\begin{array}{c}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3} \\
\vdots \\
\Psi_{n}
\end{array}\right] \text { and } \Psi_{a}=\left[\begin{array}{llllll}
a_{1} & a_{2} & a_{3} & \cdots & a_{n}
\end{array}\right]\left[\begin{array}{c}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3} \\
\vdots \\
\Psi_{n}
\end{array}\right]
\end{gathered}
$$

$$
\text { but since } \Psi_{a}=\xi_{o p} \Psi_{c}
$$

$$
\left[\begin{array}{c}
a_{1} \\
a_{2} \\
a_{3} \\
\vdots \\
a_{n}
\end{array}\right]=\left[\begin{array}{ccccc}
\xi_{11} & \xi_{12} & \xi_{13} & \cdots & \xi_{1 n} \\
\xi_{21} & \xi_{22} & \cdots & & \xi_{2 n} \\
\xi_{31} & \vdots & \ddots & & \\
\vdots & & & \ddots & \\
\xi_{n 1} & & & & \xi_{n n}
\end{array}\right]\left[\begin{array}{c}
c_{1} \\
c_{2} \\
c_{3} \\
\vdots \\
c_{n}
\end{array}\right]
$$

## Matrix Methods in Quantum Mechanics

But how do we find the individual matrix elements $\xi_{i j}$ ? Consider our two states $\Psi_{c}$ and $\Psi_{a}$ :
$\Psi_{\mathrm{a}}=\xi_{\mathrm{op}} \Psi_{\mathrm{c}}$ where $\Psi_{\mathrm{c}}=\sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}$ and $\Psi_{\mathrm{a}}=\sum_{\mathrm{i}} \mathrm{a}_{\mathrm{i}} \Psi_{\mathrm{i}}$
Applying the operator, $\quad \Psi_{\mathrm{a}}=\xi_{o p} \sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}$
Multiplying both sides by $\Psi_{j}^{*}$ and integrating over all space,

$$
\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \Psi_{\mathrm{a}} d v=\sum_{\mathrm{i}} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p}\left(\mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}\right) d v
$$

Now subtituting in for $\Psi_{c}$, and only working on the left hand side,
$\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \sum_{\mathrm{i}} \mathrm{a}_{\mathrm{i}} \Psi_{\mathrm{i}} d v=\sum_{\mathrm{i}} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p}\left(\mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}\right) d v$
$\sum_{\mathrm{i}} \int_{-\infty}^{\infty} \mathrm{a}_{\mathrm{i}} \Psi_{\mathrm{j}}^{*} \Psi_{\mathrm{i}} d v=\sum_{\mathrm{i}} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p}\left(\mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}\right) d v$
$\sum_{\mathrm{i}} \mathrm{a}_{\mathrm{i}} \delta_{i j}=\sum_{\mathrm{i}} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p}\left(\mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}\right) d v$
$\mathrm{a}_{\mathrm{j}}=\sum_{\mathrm{i}} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p}\left(\mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}}\right) d v$
But the right hand side can be rewritten as,
$\mathrm{a}_{\mathrm{j}}=\sum_{\mathrm{i}}\left[\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p} \Psi_{\mathrm{i}} d v\right] \mathrm{c}_{\mathrm{i}} \quad$ or
See discussion Brennan section 1.7 for details
$\mathrm{a}_{\mathrm{j}}=\sum_{\mathrm{i}} \xi_{j i} \mathrm{c}_{\mathrm{i}}$, where $\xi_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p} \Psi_{\mathrm{i}} d v$

## Matrix Methods in Quantum Mechanics

The two state vectors can thus be related by a transformation (operator) matrix made up of matrix elements $\xi_{\mathrm{ij}}$.

$$
\begin{gathered}
\Psi_{\mathrm{c}}=\sum_{\mathrm{i}} \mathrm{c}_{\mathrm{i}} \Psi_{\mathrm{i}} \text { and } \Psi_{\mathrm{a}}=\sum_{\mathrm{i}} \mathrm{a}_{\mathrm{i}} \Psi_{\mathrm{i}} \\
\Psi_{\mathrm{c}}=\left[\begin{array}{lllll}
\mathrm{c}_{1} & \mathrm{c}_{2} & \mathrm{c}_{3} & \cdots & \mathrm{c}_{\mathrm{n}}
\end{array}\right]\left[\begin{array}{c}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3} \\
\vdots \\
\Psi_{\mathrm{n}}
\end{array}\right] \text { and } \Psi_{\mathrm{a}}=\left[\begin{array}{lllll}
\mathrm{a}_{1} & \mathrm{a}_{2} & \mathrm{a}_{3} & \cdots & \mathrm{a}_{\mathrm{n}}
\end{array}\right]\left[\begin{array}{c}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3} \\
\vdots \\
\Psi_{\mathrm{n}}
\end{array}\right]
\end{gathered}
$$

$$
\text { but since } \Psi_{\mathrm{a}}=\xi_{\mathrm{op}} \Psi_{\mathrm{c}}
$$

$$
\begin{aligned}
& {\left[\begin{array}{c}
\mathrm{a}_{1} \\
\mathrm{a}_{2} \\
\mathrm{a}_{3} \\
\vdots \\
\mathrm{a}_{\mathrm{n}}
\end{array}\right]=\left[\begin{array}{ccccc}
\xi_{11} & \xi_{12} & \xi_{13} & \cdots & \xi_{1 \mathrm{n}} \\
\xi_{21} & \xi_{22} & \cdots & & \xi_{2 \mathrm{n}} \\
\xi_{31} & \vdots & \ddots & & \\
\vdots & & & \ddots & \\
\xi_{\mathrm{n} 1} & & & & \xi_{\mathrm{nn}}
\end{array}\right]\left[\begin{array}{c}
\mathrm{c}_{1} \\
\mathrm{c}_{2} \\
\mathrm{c}_{3} \\
\vdots \\
\mathrm{c}_{\mathrm{n}}
\end{array}\right]} \\
& \mathrm{a}_{\mathrm{j}}=\sum_{\mathrm{i}} \xi_{j i} \mathrm{c}_{\mathrm{i}}, \text { where } \xi_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p} \Psi_{\mathrm{i}} d v
\end{aligned}
$$

Thus, many Quantum Mechanics problems reduce down to calculating integrals for each matrix element and then solving NUMERICAL matrix equations.

## Matrix Methods in Quantum Mechanics

Consider what happens to the operator matrix if the basis wave set are Eigenfunctions of the operator.

$$
\left[\begin{array}{c}
a_{1} \\
a_{2} \\
a_{3} \\
\vdots \\
a_{n}
\end{array}\right]=\left[\begin{array}{ccccc}
\xi_{11} & \xi_{12} & \xi_{13} & \cdots & \xi_{1 n} \\
\xi_{21} & \xi_{22} & \cdots & & \xi_{2 n} \\
\xi_{31} & \vdots & \ddots & & \\
\vdots & & & \ddots & \\
\xi_{n 1} & & & & \xi_{n n}
\end{array}\right]\left[\begin{array}{c}
c_{1} \\
c_{2} \\
c_{3} \\
\vdots \\
c_{n}
\end{array}\right]
$$



$$
\begin{gathered}
\text { where } \xi_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \xi_{o p} \Psi_{\mathrm{i}} d v \\
\xi_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \lambda_{i} \Psi_{\mathrm{i}} d v=\lambda_{i} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \Psi_{\mathrm{i}} d v=\lambda_{i} \delta_{i j}
\end{gathered}
$$

$$
\left[\begin{array}{c}
a_{1} \\
a_{2} \\
a_{3} \\
\vdots \\
a_{n}
\end{array}\right]=\left[\begin{array}{ccccc}
\left(\xi_{11}=\lambda_{1}\right) & 0 & 0 & \cdots & 0 \\
0 & \left(\xi_{22}=\lambda_{2}\right) & \cdots & & 0 \\
0 & \vdots & \left(\xi_{33}=\lambda_{3}\right) & & 0 \\
\vdots & & & \ddots & \vdots \\
0 & & & & \left(\xi_{n n}=\lambda_{n}\right)
\end{array}\right]\left[\begin{array}{c}
c_{1} \\
c_{2} \\
c_{3} \\
\vdots \\
c_{n}
\end{array}\right]
$$

Thus, using a Eigenfunction basis set results in a diagonal matrix whose elements are the Eigenvalues. Working in reverse, if we can diagonalize the matrix, we can find all the Eigenvalues along the diagonal.

## Matrix Methods in Quantum Mechanics

Consider the case of the Schrödinger Equation (described in detail in the next lecture). This equation can be written as an Eigenvalue equation of the form:

$$
\mathbf{H} \Psi=\mathbf{E} \Psi
$$

where $H$ is the Hamiltonian operator (total energy) and $E$ is the energy Eigenvalue.

Considering $\Psi$ to be a vector wave state, we can rewrite the Schrödinger Equation as,

$$
H \sum_{i} c_{i} \Psi_{i}=E \sum_{i} c_{i} \Psi_{i}
$$

Multiplying by $\Psi_{\mathrm{j}}^{*}$ and integrating over all space,

$$
\begin{aligned}
& \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \sum_{i} c_{i} \Psi_{i} d v=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} E \sum_{i} c_{i} \Psi_{i} d v \\
& \sum_{i} c_{i} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \Psi_{i} d v=\sum_{i} E c_{i} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \Psi_{i} d v
\end{aligned}
$$

defining $H_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \Psi_{\mathrm{i}} d v$ and subtracting the right side from the left, this becomes,

$$
\begin{gathered}
\sum_{i} c_{i} H_{i j}-\sum_{i} E c_{i} \delta_{i j}=0 \\
\sum_{i} c_{i}\left(H_{i j}-E \delta_{i j}\right)=0
\end{gathered}
$$

## Matrix Methods in Quantum Mechanics

## Continued...

$$
H \sum_{i} c_{i} \Psi_{i}=E \sum_{i} c_{i} \Psi_{i}
$$

Multiplying by $\Psi_{\mathrm{j}}^{*}$ and integrating over all space,

$$
\begin{aligned}
& \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \sum_{i} c_{i} \Psi_{i} d v=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} E \sum_{i} c_{i} \Psi_{i} d v \\
& \sum_{i} c_{i} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \Psi_{i} d v=\sum_{i} E c_{i} \int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} \Psi_{i} d v
\end{aligned}
$$

defining $H_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \Psi_{\mathrm{i}} d v$ and subtracting the right side from the left, this becomes,

$$
\begin{gathered}
\sum_{i} c_{i} H_{i j}-\sum_{i} E c_{i} \delta_{i j}=0 \\
\sum_{i} c_{i}\left(H_{i j}-E \delta_{i j}\right)=0 \\
\text { or in matrix form }
\end{gathered}
$$

$$
\left[\begin{array}{ccccc}
\left(\mathrm{H}_{11}-E\right) & \mathrm{H}_{12} & \mathrm{H}_{13} & \cdots & \mathrm{H}_{1 \mathrm{n}} \\
\mathrm{H}_{21} & \left(\mathrm{H}_{22}-E\right) & \cdots & & \mathrm{H}_{2 \mathrm{n}} \\
\mathrm{H}_{31} & \vdots & \left(\mathrm{H}_{33}-E\right) & & \mathrm{H}_{3 \mathrm{n}} \\
\vdots & & & \ddots & \vdots \\
\mathrm{H}_{\mathrm{n} 1} & & & & \left(\mathrm{H}_{\mathrm{n}}-E\right)
\end{array}\right]\left[\begin{array}{c}
\mathrm{c}_{1} \\
\mathrm{c}_{2} \\
\mathrm{c}_{3} \\
\vdots \\
\mathrm{c}_{\mathrm{n}}
\end{array}\right]=0
$$

See discussion Brennan section 1.7 for details

## Matrix Methods in Quantum Mechanics

Example: Consider the system whose Hamiltonian matrix elements,

$$
H_{j i}=\int_{-\infty}^{\infty} \Psi_{\mathrm{j}}^{*} H \Psi_{\mathrm{i}} d v
$$

evaluate to:

$$
H=\left[\begin{array}{ccc}
3 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 3
\end{array}\right]
$$

What are the possible results when the energy is measured?
Writing the $(H-E) \Psi=\mathbf{0}=>(H-E)\left(c_{1} \Psi_{1}+c_{2} \Psi_{2}+c_{3} \Psi_{3}\right)=\mathbf{0}$ matrix and solving, we get:

$$
\left[\begin{array}{ccc}
(3-E) & -1 & 0 \\
-1 & (2-E) & -1 \\
0 & -1 & (3-E)
\end{array}\right]\left[\begin{array}{c}
c_{1} \\
c_{2} \\
c_{3}
\end{array}\right]=0
$$

which has a nontrivial solution for :

$$
\operatorname{DET}\left[\begin{array}{ccc}
(3-E) & -1 & 0 \\
-1 & (2-E) & -1 \\
0 & -1 & (3-E)
\end{array}\right]=0
$$

## Matrix Methods in Quantum Mechanics

## What are the possible results when the energy is measured?

$$
\left[\begin{array}{ccc}
(3-E) & -1 & 0 \\
-1 & (2-E) & -1 \\
0 & -1 & (3-E)
\end{array}\right]\left[\begin{array}{l}
c_{1} \\
c_{2} \\
c_{3}
\end{array}\right]=0
$$

which has a nontrivial solution for :

$$
\operatorname{DET}\left[\begin{array}{ccc}
(3-E) & -1 & 0 \\
-1 & (2-E) & -1 \\
0 & -1 & (3-E)
\end{array}\right]=0
$$

Expanding by minors,

$$
\begin{aligned}
& (3-\mathrm{E})\left|\begin{array}{cc}
(2-E) & -1 \\
-1 & (3-E)
\end{array}\right|-(-1)\left|\begin{array}{cc}
-1 & 0 \\
-1 & (3-E)
\end{array}\right|+0\left|\begin{array}{cc}
-1 & 0 \\
(2-E) & -1
\end{array}\right|=0 \\
& (3-E)\left(E^{2}-5 E+4\right)=0 \\
& (3-E)(1-E)(4-E)=0 \\
& \mathrm{E}=3,1 \text {, or } 4
\end{aligned}
$$

## Matrix Methods in Quantum Mechanics

What are the corresponding Eigenvectors $\Psi_{\mathrm{A}}, \Psi_{\mathrm{B}}$, and $\Psi_{\mathrm{C}}$, for each of these energy Eigenvalues? For $\mathrm{E}=1$,

$$
\left[\begin{array}{ccc}
(3-1) & -1 & 0 \\
-1 & (2-1) & -1 \\
0 & -1 & (3-1)
\end{array}\right]\left[\begin{array}{c}
c_{1} \\
c_{2} \\
c_{3}
\end{array}\right]=0
$$

which has a solution of :

$$
\begin{aligned}
& 2 c_{1}-c_{2}+0 c_{3}=0 \\
& -c_{1}+c_{2}-c_{3}=0 \\
& 0 c_{1}-c_{2}+2 c_{3}=0
\end{aligned}
$$

Solving these 3 equations and 3 unknowns yields,

Similarly for $E=3$ and $E=4$,

See discussion Brennan section 1.7 for details

$$
\begin{aligned}
& \Psi_{A}=\left[\begin{array}{lll}
1 & 2 & 1
\end{array}\right]\left[\begin{array}{l}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3}
\end{array}\right] \\
& \mathbf{d} \mathbf{E}=\mathbf{4},
\end{aligned}
$$

## Matrix Methods in Quantum Mechanics

If the ACTUAL state of the particle is described by the vector,

$$
\Psi_{\text {actaul }}=\left[\begin{array}{lll}
2 & 3 & -2
\end{array}\right]\left[\begin{array}{l}
\Psi_{1} \\
\Psi_{2} \\
\Psi_{3}
\end{array}\right]
$$

What is the probability of each Eigen-energy (the only possible measurable values) being measured?

After we normalize the states we have previously found and the state above, we must evaluate the overlap of these states. Mathematically this is either,

$$
c_{i}=\int \Psi_{i}^{*} \Psi_{\text {Actual }} d v
$$

as described previously or:
For $i=A, B$ and $C$ or equivalently in matrix form,

$$
\mathrm{c}_{\mathrm{A}}=\Psi_{\mathrm{A}} \bullet \Psi_{\text {Actual }} \quad \mathrm{c}_{\mathrm{B}}=\Psi_{\mathrm{B}} \bullet \Psi_{\text {Actual }} \quad \mathrm{c}_{\mathrm{C}}=\Psi_{\mathrm{C}} \bullet \Psi_{\text {Actual }}
$$

## Matrix Methods in Quantum Mechanics

Normalizing each of the relevant vectors we get,
$\Psi_{\text {actal }}=\frac{1}{\sqrt{17}}\left[\begin{array}{lll}2 & 3 & -2\end{array}\right]\left[\begin{array}{l}\Psi_{1} \\ \Psi_{2} \\ \Psi_{3}\end{array}\right] \quad \Psi_{A}=\frac{1}{\sqrt{6}}\left[\begin{array}{lll}1 & 2 & 1\end{array}\right]\left[\begin{array}{l}\Psi_{1} \\ \Psi_{2} \\ \Psi_{3}\end{array}\right] \quad \Psi_{B}=\frac{1}{\sqrt{2}}\left[\begin{array}{lll}1 & 0 & -1\end{array}\right]\left[\begin{array}{l}\Psi_{1} \\ \Psi_{2} \\ \Psi_{3}\end{array}\right] \quad \Psi_{C}=\frac{1}{\sqrt{3}}\left[\begin{array}{lll}1 & -1 & 1\end{array}\right]\left[\begin{array}{l}\Psi_{1} \\ \Psi_{2} \\ \Psi_{3}\end{array}\right]$

$$
\begin{gathered}
\mathrm{c}_{\mathrm{A}}=\Psi_{\mathrm{A}} \bullet \Psi_{\text {Actalal }} \quad \mathrm{c}_{\mathrm{B}}=\Psi_{\mathrm{B}} \bullet \Psi_{\text {Actual }} \quad \mathrm{c}_{\mathrm{C}}=\Psi_{\mathrm{C}} \bullet \Psi_{\text {Actalal }} \\
\mathrm{c}_{\mathrm{A}}=\frac{1}{\sqrt{6}}\left[\begin{array}{lll}
1 & 2 & 1
\end{array}\right] \cdot \frac{1}{\sqrt{17}}\left[\begin{array}{lllll}
2 & 3 & -2
\end{array}\right] \quad \mathrm{c}_{\mathrm{B}}=\frac{1}{\sqrt{2}}\left[\begin{array}{lll}
1 & 0 & -1
\end{array}\right] \bullet \frac{1}{\sqrt{17}}\left[\begin{array}{lll}
2 & 3 & -2
\end{array}\right] \quad \mathrm{c}_{\mathrm{C}}=\frac{1}{\sqrt{3}}\left[\begin{array}{lll}
1 & -1 & 1
\end{array}\right] \bullet \frac{1}{\sqrt{17}}\left[\begin{array}{lll}
2 & 3 & -2
\end{array}\right] \\
\mathrm{c}_{\mathrm{A}}=\frac{\sqrt{6}}{\sqrt{17}}
\end{gathered} \mathrm{c}_{\mathrm{B}}=\frac{\sqrt{8}}{\sqrt{17}} \quad \mathrm{c}_{\mathrm{C}}=\frac{\sqrt{3}}{\sqrt{17}} .
$$

Thus, the probability of measuring ...
...Energy $=1$ is $\mathbf{6} / 17$
...Energy $=3$ is $8 / 17$
...Energy=4 is $3 / 17$

