Lecture 5

Vector Spaces and Linear Algebra: Vector Representation of Wave States in Hilbert Spaces

Reading:

Notes and Brennan Chapter 1.6-1.7

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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]".

Consider the case of two orthogonal wave functions (two states):

If Ψ_n and Ψ_m are orthogonal, then

$$\int_{-\infty}^{\infty} \Psi_m^* \Psi_n dv = \delta_{mn}$$

However, in general, if Ψ_n and Ψ_m are orthogonal, then nothing can be said about

$$\int_{-\infty}^{\infty} \Psi_m^* \xi_{op} \Psi_n dv \stackrel{?}{=} K \delta_{mn}$$





because ξ_{op} may rotate Ψ_n into a projection of Ψ_m . However, if Ψ_n is an Eigenfunction of ξ_{op} then

$$\int_{-\infty}^{\infty} \Psi_M^* \xi_{op} \Psi_n dv = \lambda_n \int_{-\infty}^{\infty} \Psi_M^* \Psi_n dv = \lambda_n \delta_{mn}$$

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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 x, 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 <u>Fundamental Expansion Postulate</u> states that every physical observable can be represented by a Hermitian operator with a complete basis set of Eigenfunctions, $\Psi_1, \Psi_2, \Psi_3, \dots, \Psi_n$ and every physical state Ψ can be expanded as a linear combination of Eigenstates as

$$\Psi = \sum_{i} c_i \Psi_i$$

Where each coefficient is given as:

$$c_i = \int \Psi_i^* \Psi dv$$

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 yth 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 $\mathbf{r}\cdot\mathbf{y}$

See discussion Brennan p. 42-46 for details **Georgia Tech**

Proof:

Let A_{op} be a Hermitian operator with Eigenfunctions, $\Psi_1, \Psi_2, \Psi_3, \dots, \Psi_n$ and Eigenvalues $A_1, A_2, A_3, \dots A_n$. The arbitrary physical state Ψ can be expanded as a linear combination of Eigenstates as,

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

And the expectation value, <A> is then given by,

 $\left\langle A\right\rangle = \int \Psi^* A_{op} \Psi dv$

Therefore...

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Proof (cont'd):

Now using the Eigenvalue relationship

$$\begin{split} \langle A \rangle &= \int \Psi^* A_{op} \Psi dv \\ \langle A \rangle &= \int \left(\sum_i c_i^* \Psi_i^* \right) A_{op} \left(\sum_i c_i \Psi_i \right) dv \\ \langle A \rangle &= \int \left(c_1^* \Psi_1^* + c_2^* \Psi_2^* + \dots - c_n^* \Psi_n^* \right) A_{op} \left(c_1 \Psi_1 + c_2 \Psi_2 + \dots - c_n \Psi_n \right) dv \\ & \longrightarrow \langle A \rangle &= \int \left(c_1^* \Psi_1^* + c_2^* \Psi_2^* + \dots - c_n^* \Psi_n^* \right) (c_1 A_1 \Psi_1 + c_2 A_2 \Psi_2 + \dots - c_n A_n \Psi_n) dv \\ \text{but the } c_i \text{s are just numbers and since} \\ & \int \Psi_i^* \Psi_j dv &= \delta_{ij} \\ \text{all "cross terms cancel", leading to} \\ & \langle A \rangle &= \sum_i \left(A_i |c_i|^2 \int \Psi_i^* \Psi_i dv \right) \\ \text{and since } \Psi \text{ is normalized,} \\ & \langle A \rangle &= \sum_i A_i |c_i|^2 \\ & \text{Thus, } \langle A \rangle \text{ is a weighted average of the} \\ & \text{Eigenvalues, } A_i \text{ where the weights are the } |c_i|^2 \text{ 's } \end{split}$$

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Proof (cont'd):

But how do we find the $|c_i|^2$'s? Given:

$$\Psi = \sum_{i} c_{i} \Psi_{i}$$
Multiply by $\Psi_{j}^{*} \longrightarrow \Psi_{j}^{*} \Psi = \sum_{i} c_{i} \Psi_{j}^{*} \Psi_{i}$
Integrate over all
$$\int \Psi_{j}^{*} \Psi dv = \int \left(\sum_{i} c_{i} \Psi_{j}^{*} \Psi_{i} \right) dv$$
space
$$\int \Psi_{j}^{*} \Psi dv = \sum_{i} c_{i} \delta_{ij}$$

$$\int \Psi_{j}^{*} \Psi dv = c_{i}$$

Before a measurement, the particle can be in an unidentifiable state Ψ (but is made up of a linear combination of Eigenstates). However, once measured, the particle is in a known Eigenstate, Ψ_i , with known measurable variable A_i . The term "collapsing into known state Ψ_i " is often used. The $|c_i|^2$'s are the probability of collapse (probability that a measurement corresponding to Hermitian operator A_{op} of the particle in arbitrary state Ψ will result in an observable A_i).

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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.

Distributive Addition : $\Psi_{m} + \Psi_{n} = \Psi_{n} + \Psi_{m}$ and $\Psi_{m} + (\Psi_{n} + \Psi_{1}) = (\Psi_{n} + \Psi_{m}) + \Psi_{1}$ Scalor Multiplication : $\mu(\lambda\Psi_{m}) = (\mu\lambda)\Psi_{m}$ and $\lambda(\Psi_{m} + \Psi_{n}) = \lambda\Psi_{m} + \lambda\Psi_{n}$ Existance of a Null State : $\Psi_{m} + \Psi_{o} = \Psi_{m}$ Linear Independence of all States : If all $\lambda_{i} \neq 0$ then $\sum \lambda_{i}\Psi_{i} \neq 0$ 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:

$$d = \int_{-\infty}^{\infty} \Psi_{m}^{*} \Psi_{n} dv$$
$$d = \int_{-\infty}^{\infty} (\Psi_{m}^{*}) (\Psi_{n}) dv$$
$$d = \int_{-\infty}^{\infty} \left(\sum_{i} a_{i}^{*} \Psi_{i}^{*} \right) \left(\sum_{j} b_{j} \Psi_{j} \right) dv$$
$$d = \sum_{i} \sum_{j} a_{i}^{*} b_{j} \int_{-\infty}^{\infty} \Psi_{i}^{*} \Psi_{j} dv$$

but again if we used orthogonal basis functions, Ψ_i and Ψ_i ,

$$d = \sum_{i} \sum_{j} a_{i}^{*} b_{j} \delta_{ij}$$
$$d = \sum_{i} a_{i}^{*} b_{i}$$

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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:

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

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.

The <u>Fundamental Expansion Postulate</u> can be rewritten in matrix form. Every physical observable can be represented by a Hermitian operator with a complete basis set of Eigenfunctions, Ψ_1 , Ψ_2 , Ψ_3 , ..., Ψ_n and every physical state Ψ can be expanded as a linear combination of Eigenstates as

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

$$\Psi = \begin{bmatrix} c_{1} & c_{2} & c_{3} & \cdots & c_{n} \end{bmatrix} \begin{bmatrix} \Psi_{1} \\ \Psi_{2} \\ \Psi_{3} \\ \vdots \\ \Psi_{n} \end{bmatrix}$$

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

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

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:

$$\Psi_{c} = \sum_{i} c_{i} \Psi_{i} \text{ and } \Psi_{a} = \sum_{i} a_{i} \Psi_{i}$$
$$\Psi_{c} = \begin{bmatrix} c_{1} & c_{2} & c_{3} & \cdots & c_{n} \end{bmatrix} \begin{bmatrix} \Psi_{1} \\ \Psi_{2} \\ \Psi_{3} \\ \vdots \\ \Psi_{n} \end{bmatrix} \text{ and } \Psi_{a} = \begin{bmatrix} a_{1} & a_{2} & a_{3} & \cdots & a_{n} \end{bmatrix} \begin{bmatrix} \Psi_{1} \\ \Psi_{2} \\ \Psi_{3} \\ \vdots \\ \Psi_{n} \end{bmatrix}$$

but since $\Psi_a = \xi_{op} \Psi_c$

$\begin{bmatrix} a_1 \end{bmatrix}$		ξ ₁₁	ξ_{12}	ξ_{13}	•••	ξ_{1n}	$\begin{bmatrix} \mathbf{c}_1 \end{bmatrix}$
a ₂		ξ_{21}	ξ_{22}	•••		ξ_{2n}	c ₂
a ₃	=	ξ_{31}	:	••••		-	c ₃
÷		•			•.		
a _n _		ξ_{n1}				ξ_{nn}	$\lfloor c_n \rfloor$

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But how do we find the individual matrix elements ξ_{ij} ? Consider our two states Ψ_c and Ψ_a : $\Psi_a = \xi_{op} \Psi_c$ where $\Psi_c = \sum_i c_i \Psi_i$ and $\Psi_a = \sum_i a_i \Psi_i$

Applying the operator, $\Psi_{a} = \xi_{op} \sum_{i} c_{i} \Psi_{i}$

Multiplying both sides by Ψ_{j}^{*} and integrating over all space,

$$\int_{-\infty}^{\infty} \Psi_{j}^{*} \Psi_{a} dv = \sum_{i} \int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} (c_{i} \Psi_{i}) dv$$

Now subtituting in for Ψ_c , and only working on the left hand side,

$$\int_{-\infty}^{\infty} \Psi_{j}^{*} \sum_{i} a_{i} \Psi_{i} dv = \sum_{i} \int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} (c_{i} \Psi_{i}) dv$$
$$\sum_{i} \int_{-\infty}^{\infty} a_{i} \Psi_{j}^{*} \Psi_{i} dv = \sum_{i} \int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} (c_{i} \Psi_{i}) dv$$
$$\sum_{i} a_{i} \delta_{ij} = \sum_{i} \int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} (c_{i} \Psi_{i}) dv$$
$$a_{j} = \sum_{i} \int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} (c_{i} \Psi_{i}) dv$$

But the right hand side can be rewritten as,

 $a_j = \sum \xi_{ji} c_i$, where $\xi_{ji} = \int \Psi_j^* \xi_{op} \Psi_i dv$

$$\mathbf{a}_{j} = \sum_{i} \left[\int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} \Psi_{i} dv \right] \mathbf{c}_{i} \quad \text{or}$$

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

$$\Psi_{c} = \sum_{i} c_{i} \Psi_{i} \text{ and } \Psi_{a} = \sum_{i} a_{i} \Psi_{i}$$

$$\Psi_{c} = \begin{bmatrix} c_{1} & c_{2} & c_{3} & \cdots & c_{n} \end{bmatrix} \begin{bmatrix} \Psi_{1} \\ \Psi_{2} \\ \Psi_{3} \\ \vdots \\ \Psi_{n} \end{bmatrix} \text{ and } \Psi_{a} = \begin{bmatrix} a_{1} & a_{2} & a_{3} & \cdots & a_{n} \end{bmatrix} \begin{bmatrix} \Psi_{1} \\ \Psi_{2} \\ \Psi_{2} \\ \Psi_{3} \\ \vdots \\ \Psi_{n} \end{bmatrix}$$

but since $\Psi_a = \xi_{op} \Psi_c$

$$\begin{bmatrix} \mathbf{a}_{1} \\ \mathbf{a}_{2} \\ \mathbf{a}_{3} \\ \vdots \\ \mathbf{a}_{n} \end{bmatrix} = \begin{bmatrix} \xi_{11} & \xi_{12} & \xi_{13} & \cdots & \xi_{1n} \\ \xi_{21} & \xi_{22} & \cdots & \xi_{2n} \\ \xi_{31} & \vdots & \ddots & \\ \vdots & & \ddots & \\ \xi_{n1} & & & \xi_{nn} \end{bmatrix} \begin{bmatrix} \mathbf{c}_{1} \\ \mathbf{c}_{2} \\ \mathbf{c}_{3} \\ \vdots \\ \mathbf{c}_{n} \end{bmatrix}$$
$$\mathbf{a}_{j} = \sum_{i} \xi_{ji} \mathbf{c}_{i}, \text{ where } \xi_{ji} = \int_{-\infty}^{\infty} \Psi_{j}^{*} \xi_{op} \Psi_{i} dv$$

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

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Consider what happens to the operator matrix if the basis wave set are Eigenfunctions of the operator. $\begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}$ $\begin{bmatrix} \Psi_1 \\ \Psi_2 \end{bmatrix}$

$$\begin{bmatrix} a_{1} \\ a_{2} \\ a_{3} \\ \vdots \\ a_{n} \end{bmatrix} = \begin{bmatrix} \xi_{11} & \xi_{12} & \xi_{13} & \cdots & \xi_{1n} \\ \xi_{21} & \xi_{22} & \cdots & & \xi_{2n} \\ \xi_{31} & \vdots & \ddots & \\ \vdots & & & \ddots & \\ \xi_{n1} & & & & \xi_{nn} \end{bmatrix} \begin{bmatrix} c_{1} \\ c_{2} \\ c_{3} \\ \vdots \\ c_{n} \end{bmatrix}$$

where
$$\xi_{ji} = \int_{-\infty}^{\infty} \Psi_j^* \xi_{op} \Psi_i dv$$

 $\xi_{ji} = \int_{-\infty}^{\infty} \Psi_j^* \lambda_i \Psi_i dv = \lambda_i \int_{-\infty}^{\infty} \Psi_j^* \Psi_i dv = \lambda_i \delta_{ij}$

$$\begin{bmatrix} a_{1} \\ a_{2} \\ a_{3} \\ \vdots \\ a_{n} \end{bmatrix} = \begin{bmatrix} (\xi_{11} = \lambda_{1}) & 0 & 0 & \cdots & 0 \\ 0 & (\xi_{22} = \lambda_{2}) & \cdots & 0 \\ 0 & \vdots & (\xi_{33} = \lambda_{3}) & 0 \\ \vdots & & \ddots & \vdots \\ 0 & & & (\xi_{nn} = \lambda_{n}) \end{bmatrix} \begin{bmatrix} c_{1} \\ c_{2} \\ c_{3} \\ \vdots \\ c_{n} \end{bmatrix}$$

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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. Ψ_3 : Ψ_n

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:

ΗΨ=ΕΨ

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

Considering Ψ 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 Ψ_j^* and integrating over all space,

$$\int_{-\infty}^{\infty} \Psi_j^* H \sum_i c_i \Psi_i dv = \int_{-\infty}^{\infty} \Psi_j^* E \sum_i c_i \Psi_i dv$$
$$\sum_i c_i \int_{-\infty}^{\infty} \Psi_j^* H \Psi_i dv = \sum_i E c_i \int_{-\infty}^{\infty} \Psi_j^* \Psi_i dv$$

defining $H_{ji} = \int_{-\infty}^{\infty} \Psi_j^* H \Psi_i dv$ and subtracting the right side from the left, this becomes,

$$\sum_{i} c_{i} H_{ij} - \sum_{i} E c_{i} \delta_{ij} = 0$$
$$\sum_{i} c_{i} (H_{ij} - E \delta_{ij}) = 0$$

See discussion Brennan section 1.7 for details



See discussion Brennan section 1.7 for details

Example: Consider the system whose Hamiltonian matrix elements,

$$H_{ji} = \int_{-\infty}^{\infty} \Psi_j^* H \Psi_i dv$$

evaluate to:

$$H = \begin{bmatrix} 3 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 3 \end{bmatrix}$$

What are the possible results when the energy is measured?

Writing the (H-E) $\Psi=0 \Rightarrow$ (H-E) $(c_1\Psi_1+c_2\Psi_2+c_3\Psi_3)=0$ matrix and solving, we get:

$\left\lceil (3-E) \right\rceil$	-1	0	$\begin{bmatrix} c_1 \end{bmatrix}$	
-1	(2-E)	-1	c_2	= 0
0	-1	(3-E)	$\lfloor c_3 \rfloor$	

which has a nontrivial solution for :

$$DET\begin{bmatrix} (3-E) & -1 & 0\\ -1 & (2-E) & -1\\ 0 & -1 & (3-E) \end{bmatrix} = 0$$

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What are the possible results when the energy is measured?

$$\begin{bmatrix} (3-E) & -1 & 0 \\ -1 & (2-E) & -1 \\ 0 & -1 & (3-E) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = 0$$

which has a nontrivial solution for :

$$DET\begin{bmatrix} (3-E) & -1 & 0\\ -1 & (2-E) & -1\\ 0 & -1 & (3-E) \end{bmatrix} = 0$$

Expanding by minors,

$$(3-E) \begin{vmatrix} (2-E) & -1 \\ -1 & (3-E) \end{vmatrix} - (-1) \begin{vmatrix} -1 & 0 \\ -1 & (3-E) \end{vmatrix} + 0 \begin{vmatrix} -1 & 0 \\ (2-E) & -1 \end{vmatrix} = 0 (3-E)(E^2 - 5E + 4) = 0 (3-E)(1-E)(4-E) = 0$$

$$E = 3, 1, or 4$$

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What are the corresponding Eigenvectors Ψ_A , Ψ_B , and Ψ_C , for each of these energy Eigenvalues? For E=1,

$$\begin{bmatrix} (3-1) & -1 & 0 \\ -1 & (2-1) & -1 \\ 0 & -1 & (3-1) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = 0$$

which has a solution of :

$$2c_1 - c_2 + 0c_3 = 0$$
$$-c_1 + c_2 - c_3 = 0$$
$$0c_1 - c_2 + 2c_3 = 0$$

Solving these 3 equations and 3 unknowns yields,



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

$$\Psi_{actual} = \begin{bmatrix} 2 & 3 & -2 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix}$$

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,

$$c_i = \int \Psi_i^* \Psi_{Actual} dv$$

as described previously or:

For i=A, B and C or equivalently in matrix form,

$$\mathbf{c}_{\mathrm{A}} = \Psi_{\mathrm{A}} \bullet \Psi_{\mathrm{Actual}} \qquad \mathbf{c}_{\mathrm{B}} = \Psi_{\mathrm{B}} \bullet \Psi_{\mathrm{Actual}} \qquad \mathbf{c}_{\mathrm{C}} = \Psi_{\mathrm{C}} \bullet \Psi_{\mathrm{Actual}}$$

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Normalizing each of the relevant vectors we get,

$$\Psi_{actual} = \frac{1}{\sqrt{17}} \begin{bmatrix} 2 & 3 & -2 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} \qquad \Psi_A = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} \qquad \Psi_B = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix} \qquad \Psi_C = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \end{bmatrix}$$

$$c_{A} = \Psi_{A} \bullet \Psi_{Actual} \quad c_{B} = \Psi_{B} \bullet \Psi_{Actual} \quad c_{C} = \Psi_{C} \bullet \Psi_{Actual}$$

$$c_{A} = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 & 2 & 1 \end{bmatrix} \bullet \frac{1}{\sqrt{17}} \begin{bmatrix} 2 & 3 & -2 \end{bmatrix} \quad c_{B} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} \bullet \frac{1}{\sqrt{17}} \begin{bmatrix} 2 & 3 & -2 \end{bmatrix} \quad c_{C} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & -1 & 1 \end{bmatrix} \bullet \frac{1}{\sqrt{17}} \begin{bmatrix} 2 & 3 & -2 \end{bmatrix} \quad c_{A} = \frac{\sqrt{6}}{\sqrt{17}} \quad c_{B} = \frac{\sqrt{8}}{\sqrt{17}} \quad c_{C} = \frac{\sqrt{3}}{\sqrt{17}}$$

Thus, the probability of measuring ...

See discussion Brennan section 1.7 for details