More Linear Vector Spaces

Concepts of primary interest:

- **Complex spaces**
- **Hermitian**
- **Adjoint**
- **Mapping**
- **Linear Operator**
- **Transformation**

Sample calculations:

Application examples:

Tools of the trade:

- **Cheap Legendre expansions**
- **Matthew Davis Method for Generating Matrix Representations**

This handout is a continuation of the Introduction to Vector Spaces handout. You should review that handout now.

Representations: Our vector space notation is abstract; representations lower the degree of the abstraction.

Consider the inner product. An integral representation for the inner product is used in introductory quantum mechanics.

$$\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \phi(x) \, dx$$

$$\langle \quad \psi \quad | \quad \phi \quad \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \phi(x) \, dx$$

A robust representation of the inner product includes the instructions required to *actually compute* the scalar value of the inner product.

Exercise: Show that the inner product definition $\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \phi(x) \, dx$ satisfies the four axioms for inner products.

Matrix Representation of a Linear Vector Space: Matrices may be used as a convenient representation of vectors and vector operations. A representation is anchored by the selection of a basis set for the vector space and evaluating the expansion coefficients for all the vectors using this basis. Most of the examples display three dimensions, but they could be for *N* dimensions.

Basis: Orthogonal and Unity Normalized:

Consider the vector: $|V_i\rangle = a_i |e_1\rangle + b_i |e_2\rangle + c_i |e_3\rangle$. The basis set $\{|e_1\rangle, |e_2\rangle, |e_3\rangle\}$is both orthogonal and unity normalized. The coefficients: $\{a_i, b_i, c_i\}$ are often called components. As an example, the $|e_1\rangle$ component of $|V_i\rangle$ can be **projected** out using the inner product.

$$\langle e_1 | V_i \rangle = a_i \langle e_1 | e_1 \rangle + b_i \langle e_1 | e_2 \rangle + c_i \langle e_1 | e_3 \rangle = a_i \quad \text{after using} \quad \langle e_i | e_j \rangle = \delta_{ij}$$

Once $\{|e_1\rangle, |e_2\rangle, |e_3\rangle\}$, a specific set of basis vectors, has been chosen that is orthogonal and unity normalized ($\langle e_i | e_j \rangle = \delta_{ij}$), any vector can be *uniquely* represented by the column matrix of its components. The vector is the linear combination of the basis vectors using those components, and the basis is to remain the specified set with no changes allowed. (A change of basis requires that a complex translation procedure called a transformation be invoked to relate the representation in terms of the original basis to the representation using the new basis.)

The dagger operation converts a ket to its corresponding bra and vice versa.

The Dagger† Operation:

1.) The dagger operation converts a KET vector to its corresponding (conjugate) BRA vector. That is: $|M\rangle^{\dagger} = \langle M|$.

2.) The dagger operation also converts a BRA vector to its corresponding (conjugate) KET vector.

3.) If the dagger operation is performed twice, the original vector is recovered. $\left[\left|M\right\rangle^{\dagger}\right]^{\dagger} = \left\langle M\right|^{\dagger} = \left|M\right\rangle$.

$\left[\left\langle M\right|^{\dagger}\right]^{\dagger} = \left[\left|M\right\rangle\right]^{\dagger} = \left\langle M\right|$

4.) The dagger on a BRA-KET follows as $(\left\langle I\middle|M\right\rangle)^{\dagger} = \left\langle M\middle|I\right\rangle$. The inner product of two vectors is a scalar $\langle I|M\rangle = d$ and $\left\langle I\middle|M\right\rangle = \left\langle M\middle|I\right\rangle^{*}$ so the dagger operation acting on a complex (or real) scalar returns the complex conjugate of that scalar; $(d\,)^{\dagger} = d^{*}$.

5.) Dagger operation on multiplying constants: $(d\,|M\rangle\,)^{\dagger} = |d\,M\rangle^{\dagger} = \langle d\,M| = d^{*}\,\langle M|$.

NOTE: Dagger should appear as † but font wars are leading to † and even to a superscript t (^{t}).

The details follow from the requirement that the BRA-KET combination follows the rules for the chosen inner product. Properties (I2) and (I3) of the inner product provide additional information about the action of the dagger operation.

I2. $\left\langle I\middle|\left(d\left|M\right\rangle\right)\right. = d\,\left\langle I\middle|M\right\rangle$ where d is any scalar. *Scaling*

I3. $\left\langle I\middle|M\right\rangle = \left\langle M\middle|I\right\rangle^{*}$ asterisk means complex conjugate *'Hermitian'*

$$\left\langle I\middle|d\,M\right\rangle^{*} = \left(d\left\langle I\middle|M\right\rangle\right)^{*} = d^{*}\left\langle I\middle|M\right\rangle^{*} = d^{*}\left\langle M\middle|I\right\rangle$$

and $\left\langle I\middle|d\,M\right\rangle^{*} = \left\langle dM\middle|I\right\rangle = \left\langle I\middle|d\,M\right\rangle^{\dagger} = d^{*}\left\langle M\middle|I\right\rangle$

$$\boxed{\text{The conclusion is that: } \left|d\,M\right\rangle^{\dagger} = d^{*}\left\langle M\right|.}$$

This statement is consistent with the dagger operation returning the complex conjugates of scalars. Complex conjugation and the dagger operation are distinct operations that can be used to interchange BRAs and KETs.

Exercise: Use the correspondence to the right to justify the identifications of $\|c\,M\rangle$ as $c\,\|\,M\rangle$ and of $\langle d\,M\|$ as $d^{*}\,\langle M\|$.	$\left\langle \psi \middle\| \phi \right\rangle = \int_{-\infty}^{\infty}[\psi(x)]^{*}\,\phi(x)\,dx$

***** Important Exercise:** Follow the rules above and apply the properties of the inner product to show that: $\left[\left|A\right\rangle - \dfrac{\left\langle B\middle|A\right\rangle\left|B\right\rangle}{\left\langle B\middle|B\right\rangle}\right]^{\dagger} = \left\langle A\right| - \dfrac{\left\langle A\middle|B\right\rangle\left\langle B\right|}{\left\langle B\middle|B\right\rangle}$. $\left\langle B\middle|A\right\rangle$ is a complex scalar.

If one considers $\left|C\right\rangle = \left|A\right\rangle - \dfrac{\left\langle B\middle|A\right\rangle\left|B\right\rangle}{\left\langle B\middle|B\right\rangle}$ then the condition $\left\langle C\middle|C\right\rangle \geq 0$ (inner product property I4) proves that $\left\langle A\middle|A\right\rangle\left\langle B\middle|B\right\rangle \geq \left|\left\langle A\middle|B\right\rangle\right|^{2}$ which is the Schwarz inequality.

Digression: Why is $|C\rangle = |A\rangle - \frac{\langle B|A\rangle|B\rangle}{\langle B|B\rangle}$ important? First consider the analogous expression in a more familiar setting. $\vec{C} = \vec{A} - \frac{(\vec{B}\cdot\vec{A})\,\vec{B}}{(\vec{B}\cdot\vec{B})} = \vec{A} - (\hat{B}\cdot\vec{A})\,\hat{B}$. Start with $\vec{A}$ and compute the component of $\vec{A}$ in the direction of $\vec{B}$ which is $(\hat{B}\cdot\vec{A})\,\hat{B}$. The vector $\vec{C}$ is what remains of $\vec{A}$ after the part parallel to $\vec{B}$ has been removed. What can be said about $\vec{C}$ and $\vec{B}$? What can be said about their directions?

In the abstract setting, it follows that $|C\rangle$ is what remains of $|A\rangle$ after its behavior $|B\rangle$ behavior has been removed. That is: Start with $|A\rangle$; remove all the $|B\rangle$ behavior in $|A\rangle$; the remainder $|C\rangle$ is orthogonal to $|B\rangle$ as it has no $|B\rangle$ behavior.

The Dagger Operation in the matrix representation:

$$|V_i\rangle \rightarrow \begin{bmatrix} a_i \\ b_i \\ c_i \end{bmatrix} \qquad \text{and} \qquad |V_j\rangle^\dagger = \langle V_j| \rightarrow \begin{bmatrix} a_j^* & b_j^* & c_j^* \end{bmatrix}$$

Dagger in matrix rep $\Rightarrow$ Complex conjugate of the transpose

The actual vector is $|V_i\rangle = a_i|\hat{e}_1\rangle + b_i|\hat{e}_2\rangle + c_i|\hat{e}_3\rangle$, but the basis vectors need not be displayed ***as long as*** that basis set is specified and understood to be immutable.

A robust representation is capable of supporting all the rules followed by the vectors. Addition is the standard matrix addition. Scalar multiplication is the standard scalar multiplication for matrices. The **DAGGER Operation** (converting kets to bras and vice versa) is the complex conjugation of the transpose. Finally, the inner product is realized as matrix multiplication of the bra and ket.

$$\langle V_j|V_i\rangle = \begin{bmatrix} a_j^* & b_j^* & c_j^* \end{bmatrix} \begin{bmatrix} a_i \\ b_i \\ c_i \end{bmatrix} = a_j^* a_i + b_j^* b_i + c_j^* c_i$$

Inner Product $\Rightarrow$ Matrix Product

The procedures above were relative straight forward.

Alternatives to an orthonormal basis that we will attempt to avoid.

Basis: Orthogonal and normalized (not unity normalized)

A basis expansion set is chosen to be three orthogonal vectors that are not unity normalized.

$$\left|V_i\right\rangle = c_{1i}\left|b_1\right\rangle + c_{2i}\left|b_2\right\rangle + c_{3i}\left|b_3\right\rangle \quad \text{where } \left\langle b_i \middle| b_j\right\rangle = N_j\ \delta_{ij}$$

As above,

$$\left|V_i\right\rangle \rightarrow \begin{bmatrix} c_{1i} \\ c_{2i} \\ c_{3i} \end{bmatrix} \quad \text{and} \quad \left\langle V_j\right| \rightarrow \begin{bmatrix} c_{1j}^* & c_{2j}^* & c_{3j}^* \end{bmatrix}$$

but the inner product is rather more complicated:

$$\begin{aligned}\left\langle V_j \middle| V_i\right\rangle &= \left(c_{1j}^*\left\langle b_1\right| + c_{2j}^*\left\langle b_2\right| + c_{3j}^*\left\langle b_3\right|\right)\left(c_{1i}\left|b_1\right\rangle + c_{2i}\left|b_2\right\rangle + c_{3i}\left|b_3\right\rangle\right) \\ &= \left(c_{1j}^*\ c_{1i}\left\langle b_1 \middle| b_1\right\rangle + c_{2j}^*\ c_{2i}\left\langle b_2 \middle| b_2\right\rangle + c_{3j}^*\ c_{3i}\left\langle b_3 \middle| b_3\right\rangle\right) = c_{1j}^*\ c_{1i}N_1 + c_{2j}^*\ c_{2i}N_2 + c_{3j}^*\ c_{3i}N_3\end{aligned}$$

$$\left\langle V_j \middle| V_i\right\rangle = \begin{bmatrix} c_{1j}^* & c_{2j}^* & c_{3j}^* \end{bmatrix}\begin{bmatrix} N_1 & 0 & 0 \\ 0 & N_2 & 0 \\ 0 & 0 & N_3 \end{bmatrix}\begin{bmatrix} c_{1i} \\ c_{2i} \\ c_{3i} \end{bmatrix} = c_{1j}^* c_{1i}\ N_1 + c_{2j}^* c_{2i}\ N_2 + c_{3j}^* c_{3i}\ N_3$$

Basis: Just linearly independent (not orthogonal or unity normalized)

A basis expansion set is chosen to be three ***linearly independent*** vectors $\{s_1, s_2, s_3\}$ which are neither orthogonal nor unity normalized.

$$\left|V_i\right\rangle = c_{1i}\left|s_1\right\rangle + c_{2i}\left|s_2\right\rangle + c_{3i}\left|s_3\right\rangle$$

As the basis is not mutually orthogonal, any $\langle s_i|\ s_j\rangle$ can be non-zero. Define $\left\langle s_i \middle| s_j\right\rangle = n_{ij}$.

$$\left|V_i\right\rangle \rightarrow \begin{bmatrix} c_{1i} \\ c_{2i} \\ c_{3i} \end{bmatrix} \quad \text{and} \quad \left\langle V_j\right| \rightarrow \begin{bmatrix} c_{1j}^* & c_{2j}^* & c_{3j}^* \end{bmatrix}$$

A vector has a unique expansion in terms of any linearly independent basis set. The values for (c_{1i}, c_{2i}, c_{3i}) for a vector are unique for a given basis set which, by definition is a set of linearly independent vectors.

The inner product is much more complicated: $n_{ij} = \left\langle s_i \middle| s_j \right\rangle$

$$\left\langle V_j \middle| V_i \right\rangle = \begin{bmatrix} c_{1j}^* & c_{2j}^* & c_{3j}^* \end{bmatrix} \begin{bmatrix} n_{11} & n_{21} & n_{31} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{bmatrix} \begin{bmatrix} c_{1i} \\ c_{2i} \\ c_{3i} \end{bmatrix} = \sum_{i,j=1}^{3} c_{\ell j}^* n_{\ell m} c_{mi}$$

The moral is to work hard when you build your basis. Make sure that it is orthogonal and unity normalized. At the very least, make sure that the basis is orthogonal.

The expansion basis for Fourier series is orthogonal, but not unity normalized.

$$\frac{1}{T}\int_{-T/2}^{T/2} [1]\ [1]\, dt = 1; \qquad \frac{1}{T}\int_{-T/2}^{T/2} [1] \sin[\omega_m t]\, dt = 0; \qquad \frac{1}{T}\int_{-T/2}^{T/2} [1] \cos[\omega_m t]\, dt = 0$$

$$\frac{1}{T}\int_{-T/2}^{T/2} \sin[\omega_p t] \cos[\omega_m t]\, dt = 0; \quad \frac{1}{T}\int_{-T/2}^{T/2} \sin[\omega_p t] \sin[\omega_m t]\, dt = ½\, \delta_{pm}; \quad \frac{1}{T}\int_{-T/2}^{T/2} \cos[\omega_p t] \cos[\omega_m t]\, dt = ½\, \delta_{pm}$$

The sines and cosines are normalized to an inner product value of ½.

Mappings, Operators[1] and Transformations:

A vector-to-vector mapping associates each vector in a space $\mathbb{V}$ with a vector in a space $\mathbb{W}$. An operator is a mapping that associates each vector in a space $\mathbb{V}$ with a vector in the same space $\mathbb{V}$.

A mapping might associate the triplet (a_1, a_2, a_3) with the Fourier series space vector

[1] The definitions of the terms mapping, operator and transformation used in these handouts are not the standards in all fields. You should review their definitions critically when you encounter the terms in other contexts.

$$f(t) = (a_1 + a_2 + a_3) + \sum_{k=1}^{\infty} a_1^k \cos([3k-2]\omega_0 t) + a_2^k \cos([3k-1]\omega_0 t) + a_3^k \cos(3k\omega_0 t).$$

An operator might map a function (vector) in the space of infinitely differentiable functions to yield another infinitely differentiable function, another member of the same space. An operator acts on a vector to return another (perhaps/usually distinct) vector ***in the same space***. A mapping associates each vector in a space $\mathbb{V}$ with a vector in a *potentially* different space $\mathbb{W}$.

An operator yields a vector in the same space; it associates each vector in the space $\mathbb{V}$ with a vector in the space $\mathbb{V}$.

Transformations vs. Operations: Vector spaces can be represented by the collections of column vectors of the expansion coefficients for each vector in terms of a basis set. If the basis set for the expansion is changed, the particular form of a column vector representing a vector $|V_i\rangle$ changes. We will refer the changes of form due to a change in the chosen basis set as transformations. The vectors do not change, just their column vector representations. This terminology is not universal. The definitions for operator and transformation are established for use in this handout to make the cases distinct in spite of the similarities in the mechanics employed.

A **linear operator** $\hat{L}$ maps a vector into a vector in the same space $\hat{L}[|v_k\rangle] = |v_{Lk}\rangle$ where both of the vectors $|v_k\rangle$ and $|v_{Lk}\rangle$ are in the same space $\mathbb{V}$, and it has the property that:

$$\hat{L}[a|v_j\rangle + b|v_k\rangle] = a\,\hat{L}[|v_j\rangle] + b\,\hat{L}[|v_k\rangle]; \qquad a \text{ and } b \text{ are scalars}$$

Linear operators map a space $\mathbb{V}$ into a subspace of that space. In this context, the entire space $\mathbb{V}$ is one of the subspaces of the complete space $\mathbb{V}$. $(\mathbb{V} \subseteq \mathbb{V})$

Example: the derivative and the space of infinitely differentiable functions. In this case, $\hat{L} = {}^{d}/_{dx}$.

$${}^{d}/_{dx}\{a\,f(x) + b\,g(x)\} = a\,{}^{df}/_{dx} + b\,{}^{dg}/_{dx} \qquad (\checkmark)$$

The derivative is a linear operator as ${}^{df}/_{dx}$ and ${}^{dg}/_{dx}$ are infinitely differentiable functions if $f(x)$ and $g(x)$ are infinitely-differentiable, so the result is another function in the same space of functions.

For our standard three-dimensional space, rotations about the origin and projection into the *x*-*y* plane are examples of linear operations. Quantum mechanics has linear operators for the energy (the hamiltonian and $i\hbar\frac{\partial}{\partial t}$), momentum ($-i\hbar\vec{\nabla}$), position ($\vec{r}$) and many others. Each of these operates on a wavefunction to return another wavefunction (vector in the same space).

The action of a linear operator on a vector is to spit out another vector in the same space ($\hat{Q}[|\psi\rangle] = |\phi\rangle$). Consider a space with an orthonormal basis set {… ,. , $|u_k\rangle$, … }such that $\langle u_m|u_n\rangle = \delta_{mn}$. ⟨. In terms of that basis set, $|\psi\rangle = \Sigma\, a_n\, |u_n\rangle$ and $|\phi\rangle = \Sigma\, a_m\, |u_m\rangle$. Using these, the operator equation becomes:

$$\hat{Q}[|\psi\rangle] = \hat{Q}\sum_n a_n |u_n\rangle = \sum_m b_m |u_m\rangle = |\phi\rangle$$

As our operators are linear,

$$\hat{Q}\sum_n a_n |u_n\rangle = \sum_n a_n \hat{Q}|u_n\rangle = \sum_m b_m |u_m\rangle = |\phi\rangle \text{ nn}$$

In order to isolate (project out) the coefficient b_p, the expression is pre-multiplied by $\langle u_p|$, and the inner product is executed.

$$\langle u_p|\sum_n a_n \hat{Q}|u_n\rangle = \sum_n a_n \langle u_p|\hat{Q}|u_n\rangle = \sum_n \langle u_p|\hat{Q}|u_n\rangle a_n = \sum_m b_m \langle u_p|u_m\rangle = \sum_m b_m \delta_{pm} = b_p$$

The slightly larger summation in the center above is reminiscent of a matrix multiplication.

$$b_p = \Sigma_n\, Q_{pn}\, a_n$$

If we define $Q_{pn} = \langle u_p|\hat{Q}|u_n\rangle$ as the *pn* matrix element of the operator, the equation becomes:

$$|\phi\rangle = \hat{Q}|\psi\rangle \quad \rightarrow \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & \cdots \\ Q_{21} & Q_{22} & Q_{23} & \cdots \\ Q_{31} & Q_{32} & \ddots & \\ \cdots & \cdots & & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}$$

We conclude that KETs are represented as column vectors, BRAs as row vectors, inner products are row-column products and operators are matrices. Using matrix shorthand,

$$|\phi\rangle = \hat{Q}|\psi\rangle \quad \rightarrow \quad \underset{\sim}{\phi} = \underset{\approx}{Q}\,\underset{\sim}{\psi} \quad \leftrightarrow \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} & \cdots \\ Q_{21} & Q_{22} & Q_{23} & \cdots \\ Q_{31} & Q_{32} & \ddots & \\ \cdots & \cdots & & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}$$

$$\text{and } \langle \phi | \psi \rangle \quad \rightarrow \quad \underset{\sim}{\phi}^{\dagger} \underset{\sim}{\psi} \quad \leftrightarrow \quad \begin{bmatrix} b_1^* & b_2^* & b_3^* & \ldots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{bmatrix}.$$

Operating in the BRA *has not been defined*. We begin by examining a process that can move operators to the left as it interchanges the BRA and KET.

Property I3 of the inner product can be used to give:

$$\langle u_m | \hat{Q} | u_k \rangle \Rightarrow \langle u_m | \left(\hat{Q} | u_k \rangle \right) = \left\langle u_m \middle| \hat{Q} u_k \right\rangle = \left\langle \hat{Q} u_k \middle| u_m \right\rangle *$$

Complex conjugation interchanges the BRAs and the KETs, and it reveals a relation between the action of an operator on a KET and its action in a BRA.

DEFINITION: Hermitian conjugate operator (a.k.a. Adjoint Operator)[1]: One rule for moving things from BRA to KET or from KET to BRA is not enough. The adjoint of an operator is itself an operator that acts in the BRA of an inner product to yield the same result as the original operator acting in the KET. The adjoint $\hat{Q}^{\dagger}$ of an operator $\hat{Q}$ is defined by its action.

$$\left\langle \hat{Q}^{\dagger} u \middle| v \right\rangle = \left\langle u \middle| \hat{Q} v \right\rangle \quad \forall \, |u\rangle \, and \, |v\rangle \in \mathbb{V}$$

The adjoint of the operator *Q* is ***whatever it must be*** such that the adjoint operating in the BRA of an inner product yields the same result as the original operator acting in the KET.

Note that there are two processes that *move* the operator from the KET vector to the BRA vector, complex conjugation and switching to the adjoint.

An operator that is equal to its adjoint is called self-adjoint. It will have matrix representation that is Hermitian. The terms Hermitian conjugate and Hermitian are to be substituted for adjoint and self-adjoint in the remainder of this handout. A formal introduction to Hilbert spaces and the mathematics

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[1] As you read conjugate or adjoint just think of joined with, jointed to or associated with as a first step. Let the details of the relationship grow sharper as you encounter the concepts repeatedly. The adjoint of an operator *A* is also sometimes called the **Hermitian adjoint** (or conjugate *after Charles Hermite*) of *A*.

underlying quantum mechanics is appropriate to support the study of quantum mechanics in graduate school. Wait until graduate school to sort out the details.

The mathematical concept of a Hilbert space, named after David Hilbert, generalizes the notion of Euclidean space. It extends the methods of vector algebra and calculus from the two-dimensional and three-dimensional spaces to spaces with any finite or infinite number of dimensions. A Hilbert space is an abstract vector space together with the additional structure of an inner product that allows length and angle to be measured. Hilbert spaces are in addition required to be complete, a property that stipulates the existence of enough limits in the space to allow the techniques of calculus to be used.

A particular inner product is defined as: $\langle \psi | \phi \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \phi(x) \, dx$. Consider the operator x. What is its Hermitian conjugate?

$$\langle \psi | x\phi \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \{x\phi(x)\} \, dx = \langle x^\dagger \psi | \phi \rangle = \int_{-\infty}^{\infty} [x^\dagger \psi(x)]^* \, \phi(x) \, dx$$

Clearly it all works for $x^\dagger \equiv x$. It follows that $[f(x)]^\dagger = f(x)$ for all real valued functions $f(x)$. This group includes the standard potential functions encountered in a first quantum mechanics course.
What happens if a derivative is tried?

$$\langle \psi | x\phi \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \{\tfrac{d}{dx}\phi(x)\} \, dx = \left[\psi(x)^* \, \phi(x)\right]\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} [\tfrac{d}{dx}\psi(x)]^* \, \phi(x) \, dx$$

If the boundary condition $\left[\psi(x)^* \, \phi(x)\right]\Big|_{-\infty}^{\infty} = 0$ is imposed then $-\,{}^{d}/_{dx}$ is the Hermitian conjugate of ${}^{d}/_{dx}$.

$$({}^{d}/_{dx})^\dagger = -\,{}^{d}/_{dx}$$

The first thing to observe is that the Hermitian conjugate of an operator is not necessarily equal to that operator. In quantum mechanics, most of the operators that you encounter in your first course are equal to their Hermitian conjugates. Operators that are the own Hermitian conjugates are designated as Hermitian operators.

Try $-\,i\,{}^{d}/_{dx}$:

$$\langle \psi | x\phi \rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \, \{-i\tfrac{d}{dx}\phi(x)\} \, dx = \left[\psi(x)^* \, \phi(x)\right]\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \left(-i\tfrac{d}{dx}([\psi(x)]^*)\right) \phi(x) \, dx$$

$$= \left[\psi(x)^* \, \phi(x)\right]\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} [-i\tfrac{d}{dx}\psi(x)]^* \, \phi(x) \, dx$$

The operator $-\,i\,{}^{d}/_{dx}$ is its own Hermitian conjugate as is $+\,i\,{}^{d}/_{dx}$. For functions of several variables, we

would find that - $i\,{}^{\partial}/_{\partial x}$ is its own Hermitian.

Being Hermitian is a curious property, but it does prove to be useful, even crucial.

The boundary condition requirement $\left[\psi(x)^*\,\phi(x)\right]\Big|_{-\infty}^{\infty} = 0$ should be verified. It is satisfied by wavefunctions that are normalizable. ($\langle\psi|\psi\rangle = \int_{-\infty}^{\infty}[\psi(x)]^*\,\psi(x)\,dx = \text{finite}$) so we can just assume its satisfied for all localized bound state problems. It should be compared to the more general boundary condition that is required for Strum-Liouville problems ($p(x)\left[y_n(x)\dfrac{dy_m^*}{dx} - y_m^*(x)\dfrac{dy_n}{dx}\right]_a^b = 0$).

Eigenvectors and Eigenvalues: In special cases, an operator maps a vector into a scalar multiple of that same vector. This behavior is represented by the equation: $\hat{H}\,|u_k\rangle = \varepsilon_k\,|u_k\rangle$ where the $|u_k\rangle$ are the eigenvectors and the ε_k are the eigenvalues. The eigenvalues of Hermitian operators are special; they are real numbers and, as such, can represent *all the possible* results of the physical measurement associated with the operator.

$$\text{Hermitian Operator } \Rightarrow \hat{H}^\dagger \equiv \hat{H}$$

Proof: The $|u_k\rangle$ are to be *unity* normalized.

$$\hat{H}\,|u_k\rangle = \varepsilon_k\,|u_k\rangle \qquad \langle u_k|u_k\rangle = 1$$

$$\Rightarrow \langle u_k|\hat{H}|u_k\rangle = \left\langle u_k\middle|\hat{H}\,u_k\right\rangle = \varepsilon_k\,\langle u_k|\,u_k\rangle = \varepsilon_k$$

This expression $\left\langle u_k\middle|\hat{H}^\dagger u_m\right\rangle$ is to be transformed by using the defining property of the Hermitian conjugate operator to move the operator from the ket to the bra, using $\left\langle \hat{Q}^\dagger\,u\middle|v\right\rangle = \left\langle u\middle|\hat{Q}\,v\right\rangle$, and finally by moving the operator back to the ket side using I3, the complex conjugation property of the inner product.

$$\left\langle u_k\middle|\hat{H}\;u_m\right\rangle = \varepsilon_m\,\langle u_k|u_m\rangle = \left\langle \hat{H}^\dagger\,u_k\middle|u_m\right\rangle = \left\langle u_m\middle|\hat{H}^\dagger u_k\right\rangle^* = \left\langle u_k\middle|\hat{H}u_k\right\rangle^* = \varepsilon_k{}^*\langle u_m|u_k\rangle^* = \varepsilon_k{}^*\langle u_k|u_m\rangle$$

Collecting the parts with eigenvalues,

$$\varepsilon_m\,\langle u_k|u_m\rangle = \varepsilon_k{}^*\langle u_k|u_m\rangle \quad \Rightarrow \quad (\,\varepsilon_m - \varepsilon_k{}^*)\langle u_k|u_m\rangle = 0$$

The eigenvalues of a Hermitian operator are real. Choose $m = k$.

$$\left(\varepsilon_m - \varepsilon_m{}^*\right)\left\langle u_k \middle| u_m \right\rangle = \left(\varepsilon_m - \varepsilon_m{}^*\right)(1) = 0$$

The eigenvalues are equal to their own complex conjugates. They are real values.

Eigenvectors of Hermitian Operators with distinct eigenvalues are orthogonal:

$$\left(\varepsilon_m - \varepsilon_k{}^*\right)\left\langle u_k \middle| u_m \right\rangle \underset{\varepsilon_k\ real}{\rightarrow} \left(\varepsilon_m - \varepsilon_k\right)\left\langle u_k \middle| u_m \right\rangle = 0$$

The eigenvalues are assumed to be distinct, and they have been proven to be real so: $(\varepsilon_m - \varepsilon_k) \neq 0$ $\Rightarrow$ $(\varepsilon_m - \varepsilon_k{}^*) = (\varepsilon_m - \varepsilon_k) \neq 0$. It follows that the inner product of the two eigenvectors must vanish ($\left\langle u_k \middle| u_m \right\rangle = 0$) which, by definition, means that they are orthogonal

The eigenvalues of a Hermitian operator are real, and eigenvectors corresponding to distinct eigenvalues are orthogonal. The eigenvectors associated with degenerate (repeated) eigenvalues can be chosen to be orthogonal. That is: a process such as the Gram-Schmidt technique can be implemented to generate an orthogonal set from the collection of vectors that share a single eigenvalue.

The Hermitian Buzz: Hermitian operators have real eigenvalues and hence real expectation values so Hermitian operators can represent observables in quantum mechanics. Every Hermitian operator has a complete set of eigenvectors that can be used as a basis set for the space. The matrix representation of a Hermitian operator in terms of its eigen-set is diagonal. In QM, physical measurements are represented by Hermitian operators, and each Hermitian operator has a complete set of eigenfunctions that can serve as a basis set for all the physical solutions of the quantum system. The eigenvalues are the only results possible for the measurement represented by the operator.

More on Notation: A more economical notation is to be adopted for the eigenvectors of the H-operator. $\hat{H}\left|u_k\right\rangle = \varepsilon_k \left|u_k\right\rangle \rightarrow \hat{H}\left|k\right\rangle = \varepsilon_k \left|k\right\rangle$ It happens that a collection of all the eigenvectors for a Hermitian operator constitutes a basis set for the relevant vector space. The vectors in this set can be chosen to be mutually orthogonal and unity normalized. Every vector in the space can be represented as a linear combination of the basis set, $\left|v_j\right\rangle = \sum_k a_{jk}\left|k\right\rangle$. The coefficient a_{mk} can be found by projecting out the $|m\rangle$ behavior using the inner product. To do this, the equation is multiplied by the

associated bra $\langle m|$ and the inner product is executed.

$$\langle m|v_j\rangle = \sum_k a_{jk}\langle m|k\rangle = \sum_k a_{jk}\,\delta_{mk} = a_{jm} \;\; or\; a_{jm} = \langle m|v_j\rangle$$

Substituting this result into the expansion,

$$|v_j\rangle = \sum_k a_{jk}|k\rangle = \sum_k |k\rangle a_{jk} = \sum_k |k\rangle\langle k|v_j\rangle = \{\sum_k |k\rangle\langle k|\}|v_j\rangle .$$

The conclusion is that $\{\sum_k |k\rangle\langle k|\}$ = 1. A sum over KET-BRAs for all states *in a* ***complete*** *ortho-normal basis set* can be inserted into an expression at any time because it equals 1. The set of all energy eigenfunctions for a quantum problem is almost always such a complete set. After Gram-Schmidt, it will be a complete, orthonormal basis.

For example: $\langle\psi|\hat{H}\,\phi\rangle = \int_{-\infty}^{\infty}[\psi(x)]^*\,\{\hat{H}\,\phi(x)\}\,dx = \sum_{m,k}\langle\psi|m\rangle\langle m|\hat{H}|k\rangle\langle k|\phi\rangle$. Following the previous paragraph, $\langle k|\phi\rangle = a_{\phi k}$ and $\langle\psi|m\rangle = \langle m|\psi\rangle* = (a_{\psi m})*$. Defining the *matrix element* of H as: $H_{mk} = \langle m|\hat{H}|k\rangle = \int_{-\infty}^{\infty}[u_m(x)]^*\,\{\hat{H}\,u_n(x)\}\,dx$, the inner product:

$$\langle\psi|\hat{H}\,\phi\rangle = \int_{-\infty}^{\infty}[\psi(x)]^*\,\{\hat{H}\,\phi(x)\}\,dx$$

$$= \int_{-\infty}^{\infty}[\sum_m a_{\psi m}\,u_m(x))]^*\,\{\hat{H}\sum_k a_{\phi k}\,u_k(x))\}\,dx = \sum_{m,k} a^*_{\psi m} H_{mk} a_{\phi k}$$

can be cast in a matrix form.

$$\langle\psi|\hat{H}\,\phi\rangle = \begin{bmatrix} a^*_{\psi 1} & a^*_{\psi 2} & \dots & a^*_{\psi N}\end{bmatrix}\begin{bmatrix} H_{11} & H_{12} & \dots & H_{1N} \\ H_{21} & \dots & & \vdots \\ \vdots & & \ddots & \\ H_{1N} & \dots & \dots & H_{NN}\end{bmatrix}\begin{bmatrix} a_{\phi 1} \\ a_{\phi 2} \\ \vdots \\ a_{\phi N}\end{bmatrix}$$

Define: operator *matrix element* $H_{mk} = \langle m|\hat{H}|k\rangle = \int_{-\infty}^{\infty}[u_m(x)]^*\,\{\hat{H}\,u_n(x)\}\,dx$

Once a basis set has been identified, only the column vector of expansion coefficients is needed to specify a particular vector. The action of an operator is to map or transform one vector into another vector in the same space. That vector is likewise represented by its column vector of expansion coefficients in terms of the basis.

This result is valid for general operators as no special property of H has been invoked. For $\hat{O}$,

$$\left\langle \psi \middle| \hat{O}\,\phi \right\rangle = \int_{-\infty}^{\infty} [\psi(x)]^* \{\hat{O}\,\phi(x)\}\,dx = \begin{bmatrix} a_{\psi 1}^* & a_{\psi 2}^* & \dots & a_{\psi N}^* \end{bmatrix} \begin{bmatrix} O_{11} & O_{12} & \dots & O_{1N} \\ O_{21} & \dots & & \vdots \\ \vdots & & \ddots & \\ O_{1N} & \dots & \dots & O_{NN} \end{bmatrix} \begin{bmatrix} a_{\phi 1} \\ a_{\phi 2} \\ \vdots \\ a_{\phi N} \end{bmatrix}$$

$$\boxed{\text{the } \textit{matrix element}\text{: } O_{mk} = \left\langle m \middle| \hat{O} \middle| k \right\rangle = \left\langle m \middle| \hat{O}\ k \right\rangle = \int_{-\infty}^{\infty} [u_m(x)]^* \{\hat{O}\,u_n(x)\}\,dx}$$

Note that the bra contents go in the brackets [] and the ket contents go into the braces {}.

An even *more exciting* result follows as the $|k\rangle$ are eigenvectors of H.

$$\left\langle \psi \middle| \hat{H}\,\phi \right\rangle = \begin{bmatrix} a_{\psi 1}^* & a_{\psi 2}^* & \dots & a_{\psi N}^* \end{bmatrix} \begin{bmatrix} \varepsilon_1 & 0 & \dots & 0 \\ 0 & \varepsilon_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \dots & \dots & 0 \end{bmatrix} \begin{bmatrix} a_{\phi 1} \\ a_{\phi 2} \\ \vdots \\ a_{\phi N} \end{bmatrix} \quad \text{as } \hat{H}\left|k\right\rangle = \varepsilon_k \left|k\right\rangle$$

$$\left\langle \psi \middle| \hat{H}\,\phi \right\rangle = \sum_k a_{\psi k}^*\, a_{\phi k}\, \varepsilon_k \quad \text{and} \quad \left\langle \psi \middle| \hat{H}\,\psi \right\rangle = \sum_k a_{\psi k}^*\, a_{\psi k}\, \varepsilon_k$$

The final result is a compact representation for the expectation value of the energy of the quantum state $|\psi\rangle$. It supports the identifications of the $a_{\psi k}$ as a probability amplitude and the factor $(a_{\psi k})^* a_{\psi k} = |a_{\psi k}|^2$ as the probability to find the energy value ε_k as the result of a measurement on the system described by $|\psi\rangle$. In a sense the equation $\left\langle \psi \middle| \hat{H}\,\psi \right\rangle = \sum_k a_{\psi k}^*\, a_{\psi k}\, \varepsilon_k$ can be read as: the expectation value of the energy is the sum of the probabilities to find the system in each eigenstate of energy as a result of the measurement times the energy of that eigenstate. There are some subtleties for cases in which more than one state has a particular energy eigenvalue.

The states $|\psi\rangle$ and $|\phi\rangle$ that appear below are not related to the states with the same labels in the previous paragraph.

$$\left|\phi\right\rangle = \begin{bmatrix} a_{\phi 1} \\ a_{\phi 2} \\ \vdots \\ a_{\phi N} \end{bmatrix} \qquad ; \left|\psi\right\rangle = \hat{O}\left|\phi\right\rangle \quad ; \quad \left|\psi\right\rangle = \begin{bmatrix} a_{\psi 1} \\ a_{\psi 2} \\ \vdots \\ a_{\psi N} \end{bmatrix}$$

$$|\phi\rangle = \sum_k a_{\phi k}|u_k\rangle = \sum_k a_{\phi k}|k\rangle; \qquad |\psi\rangle = \sum_k a_{\psi k}|u_k\rangle = \hat{O}|\phi\rangle = \hat{O}\sum_n a_{\phi n}|u_n\rangle = \hat{O}\sum_n a_{\phi n}|n\rangle$$

The statement is that the operator acts on the states $|\phi\rangle$ to return $|\psi\rangle$, another state in the same space. Both $|\phi\rangle$ to return $|\psi\rangle$ can be represented as linear combinations of the basis vectors. The coefficient $a_{\psi m}$ can by found by projecting the $|m\rangle$ behavior out of $\hat{O}|\phi\rangle$. First, the equation is multiplied by the BRA for m behavior ($\langle m|$) and the ortho-normality property of the basis set is exercised.

$$\langle u_m|\psi\rangle = \sum_k a_{\psi k}\langle m|k\rangle = a_{\psi m} = \langle m|\hat{O}|\phi\rangle = \langle m|\hat{O}\sum_n a_{\phi n}|n\rangle = \sum_n \langle m|\hat{O}|n\rangle a_{\phi n} = \sum_n O_{mn}\, a_{\phi n}$$

The result becomes: $a_{\psi m} = \sum_n O_{mn}\, a_{\phi n}$ which is a matrix product of the matrix that represents the operator and the column vector (N x 1 matrix) that represents the original vector.

$$|\psi\rangle = \hat{O}|\phi\rangle \Rightarrow |\psi\rangle = \begin{bmatrix} a_{\psi 1} \\ a_{\psi 2} \\ \vdots \\ a_{\psi N} \end{bmatrix} = \begin{bmatrix} \langle u_1|\hat{O}|u_1\rangle & \langle u_1|\hat{O}|u_2\rangle & & \langle u_1|\hat{O}|u_N\rangle \\ \langle u_2|\hat{O}|u_1\rangle & \langle u_2|\hat{O}|u_2\rangle & & \vdots \\ \vdots & & \ddots & \vdots \\ \cdots & \cdots & & \langle u_N|\hat{O}|u_N\rangle \end{bmatrix} \begin{bmatrix} a_{\phi 1} \\ a_{\phi 2} \\ \vdots \\ a_{\phi N} \end{bmatrix}$$

$$a_{\psi k} = \langle k|\psi\rangle = \langle k|\hat{O}|\phi\rangle = \sum_n \langle k|\hat{O}|n\rangle\langle n|\phi\rangle = \sum_n O_{kn}\, a_{\phi n}$$

This result supports the identification of a Ket-Bra over a set of basis state as being equivalent to multiplication by one.

In summary: (Once a basis set has been chosen)

(1) The matrix that represents an operator is defined as:

$$\underset{\approx}{\hat{O}} = \begin{bmatrix} \langle u_1|\hat{O}|u_1\rangle & \langle u_1|\hat{O}|u_2\rangle & & \langle u_1|\hat{O}|u_N\rangle \\ \langle u_2|\hat{O}|u_1\rangle & \langle u_2|\hat{O}|u_2\rangle & & \vdots \\ \vdots & & \ddots & \vdots \\ \cdots & \cdots & & \langle u_N|\hat{O}|u_N\rangle \end{bmatrix} \Rightarrow \left[\underset{\approx}{\hat{O}}\right]_{mn} = \langle u_m|\hat{O}|u_n\rangle$$

(2) If the operator is Hermitian,

$$\left[\underset{\approx}{\hat{O}}\right]_{mn} = \langle u_m|\hat{O}|u_n\rangle = \langle u_m|\hat{O}|u_n\rangle = \langle u_m|\hat{O}u_n\rangle = \langle \hat{O}^{\dagger}u_m|u_n\rangle = \langle \hat{O}u_m|u_n\rangle = \langle u_n|\hat{O}u_m\rangle^* = \left[\underset{\approx}{\hat{O}}\right]^*_{nm}$$

The matrix representing the operator is equal to the complex conjugate of its transpose. Hermitian operators are represented by Hermitian matrices.

(3) $\left|v_j\right\rangle = \sum_k a_{jk}\left|k\right\rangle$. The coefficient a_{mk} can be found by projecting out the $|m\rangle$ behavior using the inner product. The coefficient (probability *amplitude*) $a_{jm} = \langle m|v_j\rangle$, the $|m\rangle$ behavior in $|v_j\rangle$.

(4) The square of the probability a_{jm} amplitude $|\,a_{jm}|^2$ is *the probability* that a system described by $|v_j\rangle$ will return the measurement eigenvalue associated with the state $|m\rangle$.

(5) A sum $|m\rangle\langle m|$ over a complete orthonormal basis is equivalent to 1. $(|v_j\rangle = |m\rangle\langle m|v_j\rangle)$

In many applications, N is infinity. Operators are represented by matrices of infinite dimension and vectors or wavefunctions by column vectors of infinite length.

See the **Matthew Davis Method**[1] (former USNA physics major) for the error-free generation of matrices representing operators in the Tools of the Trade section.

Exercise: Consider the bizarre operators defined by their actions as: $\hat{a}\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle$ and $\hat{b}\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle$ where set of states $|k\rangle$ is labeled by an integer index ($0 \le k < \infty$).

Sketch the forms of the matrices for these operators. By repeating the operations, it follows that: $\hat{a}^2\left|n\right\rangle = \sqrt{n(n-1)}\left|n-2\right\rangle$; $\hat{b}\,\hat{a}\left|n\right\rangle = n\left|n\right\rangle$ and $\hat{b}\,\hat{b}\left|n\right\rangle = \sqrt{(n+1)(n+2)}\left|n+2\right\rangle$.

What is $\hat{a}\,\hat{b}\left|n\right\rangle$? What is $(\hat{a}\,\hat{b} - \hat{b}\hat{a})\left|n\right\rangle$?

For those familiar with the problem, $|0\rangle$ is the ground state of the quantum harmonic oscillator and $|n\rangle$ is the nth excited state.

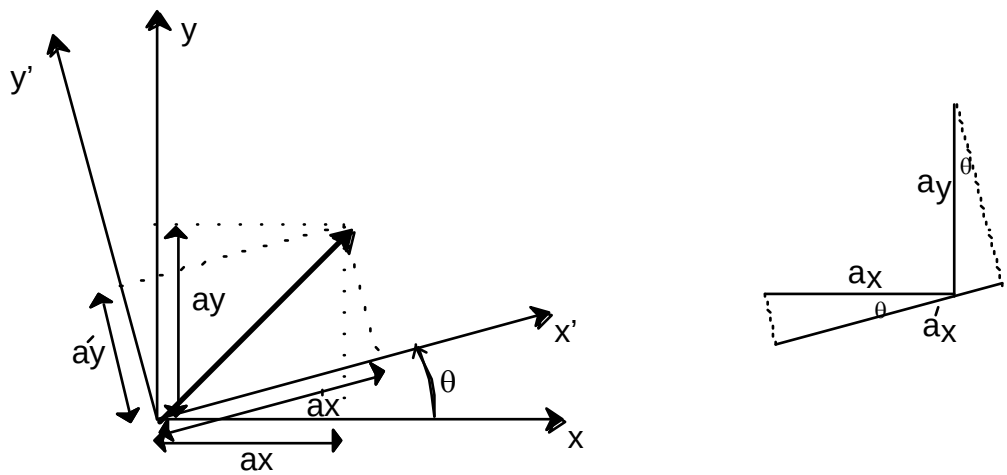
Exercise: Sketch the forms of the matrices for the operators $\hat{a}^2$; $\hat{b}\,\hat{a}$ and $(\hat{b})^2$. Show that these matrices are matrix products of the matrices for the individual operators $\hat{a}$ and $\hat{b}$.

[1] Matthew Davis is a graduate and former USNA physics major who understood that a procedure with more intermediate steps can be executed with a lower likelihood of failure due to a careless error.

The nature of physical vectors: (The discussion that follows is not complete. It only introduces some concepts for initial consideration. The reader is not expected to be convinced.) For applications in physics, one crucial additional requirement, a special transformation behavior, is added the requirements of an abstract mathematical vector space. An entity is a **physical vector** only if its representation transforms under a rotation of the coordinate axes in the same manner as does a spatial displacement, the model for a physical vector, for that same change of observer. The observer is synonymous with the reference frame or coordinate system used by that observer. Physics does not depend on the observer, and all inertial observers can make valid measurements. Physical laws are to be expressed in terms of scalars, vectors and other things (*tensors of rank 2, …* [*scalars are tensors of rank zero and vectors are tensors of rank one, a tensor of rank two is like a matrix*]) to which undergrads need not be seriously exposed. Scalars have the simplest transformation law; they stay the same. All observers report the same value for a scalar entity such as mass or temperature. Next consider a vector relation, Newton's second law $\vec{F}_{net} = m\,\vec{a}$. The mass is a scalar and so is identical according to all observers and is said to be *invariant*. Clearly transformations such as rotations scramble the components of the vectors as reported by the different observers. The only hope for retaining the validity of Newton's law component by component is if all the vectors have their components scrambled according to the same set of rules so that equalities are preserved. All the vectors transform together and are said to *co-vary*; that is, change in unison. Hence, a collection of entities is a *physical vector* only if its representation transforms under a change of observer in the same manner as does the representation of a spatial displacement, the model for a physical vector.

A problem might involve two interacting particles with the goal being to express the force exerted on particle two by particle one. Limiting the problem to some simple classical models (one might consider the case of two particles coupled together by an ideal spring), the result could be expressed as $\vec{F}_{21}\left(\vec{r}_1, \vec{r}_2\right)$. In the trivial case in which both particles are at rest, both $\vec{r}_1$ and $\vec{r}_2$ change if the observer changes position. Clearly nothing should have changed with regard to the interaction between the particles, and it becomes clear the force should not be a function of their individual positions, $\vec{r}_1$ and $\vec{r}_2$, but rather of $\vec{r}_2 - \vec{r}_1$, the displacement from particle one to particle two which is independent of the position of the observer. Considerations along this line led to the assignment of displacements as the model for vector behavior.

Rotations about the origin are a particularly fruitful example. To set the viewpoint, a change of observer or axis is envisioned, not a rotation of the system under observation. This view in which the observer changes rather than the system under observation is the *PASSIVE* definition of a transformation. If the system were to be rotated with the observer fixed, that would be *ACTIVE*. The developments in this section are to be set in the passive view. The physical system is not to be disturbed.



After some effort, one finds that $a_x^{/} = a_x \cos\theta + a_y \sin\theta,\ a_y^{/} = a_x\left(-\sin\theta\right) + a_y \cos\theta, a_z^{/} = a_z$. The transformation for the z-component is trivial because the primed observer frame was rotated by θ about the z-axis of the original unprimed observer. The observers share a common *z* axis.

Powerful techniques such as projection facilitate the computation of transformation relations. To simplify the notation the subscripts 1, 2, 3 are to be substituted for *x*, *y*, *z*. Consider a velocity $\vec{v}$ represented in an original 'fixed' system and in a primed system rotated about the origin relative to the first. It is the representation of the velocity $\vec{v}$, its components and the coordinate directions that transform, not the physical vector $\vec{v}$. It has representations in each frame.

$$\vec{v} = v_x^{/}\,\hat{i}^{/} + v_y^{/}\,\hat{j}^{/} + v_z^{/}\,\hat{k}^{/} = v_x\,\hat{i} + v_y\,\hat{j} + v_z\,\hat{k} \quad \rightarrow \qquad \vec{v} = v_1^{/}\,\hat{i}^{/} + v_2^{/}\,\hat{j}^{/} + v_3^{/}\,\hat{k}^{/} = v_1\,\hat{i} + v_2\,\hat{j} + v_3\,\hat{k}$$

The *x* or 1 component in the primed frame is **projected** out of the sum using the inner product.

$$\hat{i}^{/}\cdot\vec{v} = \hat{i}^{/}\cdot\left(v_1^{/}\,\hat{i}^{/} + v_2^{/}\,\hat{j}^{/} + v_3^{/}\,\hat{k}^{/}\right) = \hat{i}^{/}\cdot\left(v_1\,\hat{i} + v_2\,\hat{j} + v_3\,\hat{k}\right) = v_1\left(\hat{i}^{/}\cdot\hat{i}\right) + v_2\left(\hat{i}^{/}\cdot\hat{j}\right) + v_3\left(\hat{i}^{/}\cdot\hat{k}\right)$$

Therefore: $\hat{i}^{/}\cdot\vec{v} = v_1^{/} = v_1\left(\hat{i}^{/}\cdot\hat{i}\right) + v_2\left(\hat{i}^{/}\cdot\hat{j}\right) + v_3\left(\hat{i}^{/}\cdot\hat{k}\right)$

These relations can be collected into a compact representation:

$$\begin{bmatrix} v_1^{/} \\ v_2^{/} \\ v_3^{/} \end{bmatrix} = \begin{bmatrix} \left(\hat{i}^{/} \cdot \hat{i}\right) & \left(\hat{i}^{/} \cdot \hat{j}\right) & \left(\hat{i}^{/} \cdot \hat{k}\right) \\ \left(\hat{j}^{/} \cdot \hat{i}\right) & \left(\hat{j}^{/} \cdot \hat{j}\right) & \left(\hat{j}^{/} \cdot \hat{k}\right) \\ \left(\hat{k}^{/} \cdot \hat{i}\right) & \left(\hat{k}^{/} \cdot \hat{j}\right) & \left(\hat{k}^{/} \cdot \hat{k}\right) \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

The result has the form of matrix multiplication:

$$\begin{bmatrix} v_1^{/} \\ v_2^{/} \\ v_3^{/} \end{bmatrix} = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \lambda_{13} \\ \lambda_{21} & \lambda_{22} & \lambda_{23} \\ \lambda_{31} & \lambda_{32} & \lambda_{33} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

Note that λ_{ij} is $\cos(x_i^{/}, x_j)$, the cosine of the angle between the *i* axis in the rotated system and the *j* axis in the original system which are called the direction cosines. The mechanics text by J. B. Marion and S. T. Thornton is recommended for further reading on this point. A shorter discussion can be found in section 14.8 of Taylor. That discussion includes the generalization to space-time.

Exercise: Use the identification $\lambda_{ij} = \cos(x_i^{/}, x_j)$ to develop the matrix equation appropriate for a rotation of the observer frame by θ about the z-axis. Compare with the equations below the figure above.

Note that the transformation rule is based on the rule for the transformation of the coordinate systems against which displacements are referenced. All physical vectors must use this same coordinate based rule. A simple consequence is that a vector must have as many components as the coordinate space has dimensions. Some of those components may be zero in a particular representation (coordinate system), but there are always three components for a physical vector in a three dimensional universe. This statement is not intended to conflict with the practice of restricting problems to two (or even one) dimensions with a corresponding reduction in the number of components for vectors such as force and velocity. Further, in special relativity, physicists work in a four dimension space-time vector space. Physical vectors are 4D when considered in (special) relativity and must transform according to the same Lorentz transformations that apply to coordinates differences between events (space-time intervals or displacements).

Tools of the Trade:

Expansions in terms of Legendre polynomials: The first few Legendre polynomials are:

$$P_0(x)=1\,,\quad P_1(x)=x\,,\quad P_2(x)=\tfrac{3}{2}\,x^2-\tfrac{1}{2}\,,\quad P_3(x)=\tfrac{5}{2}\,x^3-\tfrac{3}{2}\,x\,,\quad P_4(x)=\tfrac{35}{8}\,x^4-\tfrac{30}{8}\,x^2+\tfrac{3}{8}$$

The typical task is to represent x^3 as a sum of the Legendre polynomials. The standard method is to project out the coefficients.

The Long Method: First one assumes that a general expansion exists: $f(x)=\sum_{m=1}^{\infty} a_m\,P_m(x)$. The second step is to multiply by a Legendre polynomial that might be represented in the sum.

$\Rightarrow P_n(x)\,f(x)=\sum_{m=1}^{\infty} a_m\,P_n(x)\,P_m(x)$. The next step is to integrate the equation from -1 to 1.

$$\int_{-1}^{1} P_n(x)\,f(x)\,dx=\sum_{m=1}^{\infty} a_m\int_{-1}^{1} P_n(x)\,P_m(x)\,dx$$

The equation is simplified by invoking the orthogonality relation:

$$\int_{-1}^{1} P_n(x)\,P_m(x)\,dx=\frac{2\delta_{mn}}{2m+1}$$

Substituting,

$$\int_{-1}^{1} P_n(x)\,f(x)\,dx=\sum_{m=1}^{\infty} a_m\int_{-1}^{1} P_n(x)\,P_m(x)\,dx=\sum_{m=1}^{\infty} a_m\,\frac{2\delta_{mn}}{2m+1}=\frac{2}{2n+1}\,a_n$$

Rearranging

$$a_n=\frac{2n+1}{2}\int_{-1}^{1} P_n(x)\,f(x)\,dx$$

The Short Method: In practice x^n can be represented as a sum of the polynomials of order n or less. Even- or odd-ness is a distinguishing behavior. So x^3, as 3 is odd, requires only odd polynomials of order less than or equal 3.

$$x^3=a\left(P_3(x)\right)+b\left(P_1(x)\right)=a\left[\tfrac{5}{2}\,x^3-\tfrac{3}{2}\,x\right]+b\left[x\right]$$

Match the highest power first: $1\,x^3=a\left(\tfrac{5}{2}\,x^3\right)$ or $a=\tfrac{2}{5}$. This choice leaves an excess of $\tfrac{2}{5}\left(\tfrac{-3}{2}\right)x=\tfrac{-3}{5}\,x=\tfrac{-3}{5}\,P_1(x)$ which is easily remedied by adding $+\tfrac{3}{5}\,P_1(x)$. It follows that $x^3=\tfrac{2}{5}\left(P_3(x)\right)+\tfrac{3}{5}\left(P_3(x)\right)$.

In general, after the highest power n is matched, a multiple of the n - 2 polynomial is added to kill off

the x^{n-2} term. Onward to n - 4 and so on until the n = 0 or 1 term is reached, and the task is accomplished.

Matthew Davis Method for Generating Matrix Representations for the raising and lowering operators.: Use this method once or twice and then try the row-column approach introduced below.

The matrix that represents an operator is defined as:

$$\underset{\approx}{\hat{O}} = \begin{bmatrix} \langle u_1|\hat{O}|u_1\rangle & \langle u_1|\hat{O}|u_2\rangle & & \langle u_1|\hat{O}|u_N\rangle \\ \langle u_2|\hat{O}|u_1\rangle & \langle u_2|\hat{O}|u_2\rangle & & \vdots \\ \vdots & & \ddots & \vdots \\ \cdots & \cdots & & \langle u_N|\hat{O}|u_N\rangle \end{bmatrix} \Rightarrow \left[\underset{\approx}{\hat{O}}\right]_{mn} = \langle u_m|\hat{O}|u_n\rangle$$

where the set { $|u_1\rangle$, $|u_2\rangle$, ..., $|u_i\rangle$, ... , ... } is the chosen basis set for the representation of operators and vectors for the space. The Matthew Davis method is to be demonstrated in the case of the lowering operator encountered in the quantum harmonic oscillator problem. The basis set is represented as { $|0\rangle$, $|1\rangle$, ..., $|n\rangle$, ... , ... } where ($0 \le n < \infty$). (One must remember that the states rows and columns are numbered from zero for this problem.) The action of the lowering operator is $\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$ and the state vectors satisfy the ortho-normality condition $\langle n|m\rangle = \delta_{mn}$. Each matrix entry $\left[\underset{\approx}{\hat{a}}\right]_{mn}$ is $\langle m|\hat{a}|n\rangle = \langle m|\hat{a}\,n\rangle = \sqrt{n}\,\langle m|\,n-1\rangle = \sqrt{n}\,\delta_{m,n-1}$. Recognizing that many errors can be avoiding by breaking a task into a series of simple steps, the Matthew Davis method to construct matrices for raising and lowering operators uses the result $\left[\underset{\approx}{\hat{a}}\right]_{mn} = \sqrt{n}\,\delta_{m,n-1}$ to fill in a matrix for a representative array of row numbers m and column numbers n. Evaluation of the entries is postponed and treated as a separate step.

$$\hat{\underset{\approx}{a}} = \begin{array}{c} m\backslash n \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} \sqrt{0}\,\delta_{0,0-1} & \sqrt{1}\,\delta_{0,1-1} & \sqrt{2}\,\delta_{0,2-1} & \sqrt{3}\,\delta_{0,3-1} & \sqrt{4}\,\delta_{0,4-1} & \sqrt{5}\,\delta_{0,5-1} \\ \sqrt{0}\,\delta_{1,0-1} & \sqrt{1}\,\delta_{1,1-1} & \sqrt{2}\,\delta_{1,2-1} & \sqrt{3}\,\delta_{1,3-1} & \sqrt{4}\,\delta_{1,4-1} & \sqrt{5}\,\delta_{1,5-1} \\ \sqrt{0}\,\delta_{2,0-1} & \sqrt{1}\,\delta_{2,1-1} & \sqrt{2}\,\delta_{2,2-1} & \sqrt{3}\,\delta_{2,3-1} & \sqrt{4}\,\delta_{2,4-1} & \sqrt{5}\,\delta_{2,5-1} \\ \sqrt{0}\,\delta_{3,0-1} & \sqrt{1}\,\delta_{3,1-1} & \sqrt{2}\,\delta_{3,2-1} & \sqrt{3}\,\delta_{3,3-1} & \sqrt{4}\,\delta_{3,4-1} & \sqrt{5}\,\delta_{3,5-1} \\ \sqrt{0}\,\delta_{4,0-1} & \sqrt{1}\,\delta_{4,1-1} & \sqrt{2}\,\delta_{4,2-1} & \sqrt{3}\,\delta_{4,3-1} & \sqrt{4}\,\delta_{4,4-1} & \sqrt{5}\,\delta_{4,5-1} \\ \sqrt{0}\,\delta_{5,0-1} & \sqrt{1}\,\delta_{5,1-1} & \sqrt{2}\,\delta_{5,2-1} & \sqrt{3}\,\delta_{5,3-1} & \sqrt{4}\,\delta_{5,4-1} & \sqrt{5}\,\delta_{5,5-1} \end{bmatrix} \end{array}$$

Evaluation:

$$\hat{\underset{\approx}{a}} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array} \begin{array}{c} \begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & 5 \end{array} \\ \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \Rightarrow \sqrt{\text{column \#}} \text{ on the first } \textit{super diagonal}$$

Breaking a task into a sequence of simpler steps decreases the likelihood of errors.

The row-column approach: $\left[\hat{\underset{\approx}{a}}\right]_{mn} = \sqrt{n}\,\delta_{m,n-1}$ or $\left[\hat{\underset{\approx}{a}}\right]_{row,col} = \sqrt{col}\,\delta_{row,col-1}$ where *row* is the row number and *col* is the column number. The Kronecker delta ensures that all the elements are zero except for those for which the row number is one less than the column number. Each element in this set is one row above an element on the main diagonal (the elements with row number equal to the column number). That is all the non-zero entries are on the first super diagonal, and each entry on the super diagonal is the square root of the column number.

The elements with column number one less than their row number form the first sub-diagonal.

$$\begin{bmatrix} D & D^1 & D^2 & D^3 & D^4 \\ D_1 & D & D^1 & D^2 & D^3 \\ D_2 & D_1 & D & D^1 & D^2 \\ D_3 & D_2 & D_1 & D & D^1 \\ D_4 & D_3 & D_2 & D_1 & D \end{bmatrix}$$

D: diagonal element

D^n: element on the nth super diagonal

D_n: element on the nth sub-diagonal

Warm Up Problems:

VSA1. A collection of elements must have two operations defined to be a vector space. What are they? Give the vector space axioms related to each of these operations.

VSA2. Give the definition of linear dependence of a set of vectors. Use the definition to class and to justify the classification of the following sets as linearly independent or as linearly dependent. $\left\{\hat{i}, \hat{j}, 3\hat{i}+\hat{k}\right\}$, $\left\{\hat{i}, \hat{j}, 3\hat{i}-\hat{j}\right\}$, $\left\{\hat{i}-j, \hat{i}+\hat{j}\right\}$ and $\left\{\hat{i}-j, \hat{i}+\hat{j}, 3\hat{i}-3\hat{j}+\hat{k}\right\}$.

VSA3. Develop the Gram-Schmidt basis sets from: $\left\{\hat{i}, \hat{j}, 3\hat{i}+\hat{k}\right\}$, $\left\{\hat{i}, \hat{j}, 3\hat{i}-\hat{j}\right\}$, and $\left\{\hat{i}-j, \hat{i}+\hat{j}, 3\hat{i}-3\hat{j}+\hat{k}\right\}$ working with each vector in the order that it appears. Give the dimension of the space spanned in each case.

VSA4. Show that the collection of elements of the form $\left|v_1\right\rangle = a_1\,\hat{i} + b_1\,\hat{j} + c_1\,\hat{k}$ where a_i, b_i and c_i can be any real number is a vector space if addition is defined as:

$\left|v_1\right\rangle + \left|v_2\right\rangle = (a_1+a_2)\,\hat{i} + (b_1+b_2)\,\hat{j} + (c_1+c_2)\,\hat{k}$ and scalar multiplication is defined as:

$d\left|v_1\right\rangle = d\,a_1\,\hat{i} + d\,b_1\,\hat{j} + d\,c_1\,\hat{k}$ where d is any real number.

VSA5. State the axioms for an inner product. Show that an inner product defined as $\langle A|B\rangle = A_x B_x + A_y B_y + A_z B_z$ satisfies those axioms for the space of vectors of the form $A_x\hat{i} + A_y\hat{j} + A_z\hat{k}$ where A_x, A_y, and A_z can be any real number. Use $\hat{e}_i \cdot \hat{e}_j = \delta_{ij}$ where $\{\hat{i}, \hat{j}, \hat{k}\} \Leftrightarrow \{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$.

Problems:

1.) Prove that if a set of *n* (numbered 1 to *n*; left to right) *non-zero* vectors is linearly dependent, that one of the vectors can be expressed as a linear combination of the previous members (ones numbered lower). Further that member can be removed from the set without the loss of any vectors from the span of the original set of *n* vectors. You may assume that the span of any set of vectors is a vector space.

2.) Suppose that you have a space $\mathbb{V}$ which is the span of a set of *n* vectors $\{|V_1\rangle, |V_2\rangle, \ldots\ldots, |V_n\rangle\}$ and you have a set of *m* linearly independent vectors $\{|W_1\rangle, |W_2\rangle, \ldots\ldots, |W_m\rangle\} \in \mathbb{V}$. Show that the Ws can be used to replace *m* members of the original set to yield a set $\{|W_1\rangle, |W_2\rangle, \ldots\ldots, |W_m\rangle, and\ (n-m)\ of\ the\ Vs\}$ that is a spanning set for the entire space $\mathbb{V}$. Conclude that $m \le n$. APPROACH: Study the definitions of all the terms. Use the axioms and previously established results related to linear independence. Base your solution on the Replacement Lemma. When you substitute the second $|W\rangle$ into the spanning set you cast out a 'current' member. What member must you argue is not cast out? Assume that one (or more) $|W\rangle$'s remains outside the spanning set after the *n* $|V\rangle$'s have been replaced by *n* $|W\rangle$'s. What property of the $|W\rangle$'s would be contradicted?

3.) Prove that if your have a basis set $\boldsymbol{B_1}$ with *m* members and a basis set $\boldsymbol{B_2}$ with *n* members for the same space $\mathbb{V}$ then $m = n$. APPROACH: Use problem VS2.

4.) Prove that the largest number of vectors in a linearly independent set of vectors in an *n* dimensional space is *n*. That is: If you have a set of *n* +1 vectors in an *n* dimensional space, then the set must be linearly dependent. APPROACH: Use the properties of a basis set and problem VS2.

5.) Consider a spanning set $\left\{ \hat{i} + 2\,\hat{j} + \hat{k},\, 2\,\hat{i} + \hat{j} + 2\,\hat{k},\, 2\,\hat{i} - 2\,\hat{j} + 2\,\hat{k} \right\}$. Apply the Gram-Schmidt procedure to find an orthonormal (orthogonal and unity normalized) basis. What is the dimension of the space spanned by this basis set?

6.) A set has members of the form $|I\rangle = a\,|e_1\rangle + b\,|e_2\rangle + c\,|e_3\rangle$ where the constants a_i, b_i, and c_i are arbitrary real numbers, the components of the vector. Addition is defined by the relation $|I\rangle + |J\rangle = (a_i + a_j)|e_1\rangle + (b_i + b_j)|e_2\rangle + (c_i + c_j)|e_3\rangle$ and scalar multiplication by $d\,|I\rangle = (d\,a)|e_1\rangle + (d\,b)|e_2\rangle + (d\,c)|e_3\rangle$. This set satisfies the requirements to be a vector space.

a.) The basis vectors $|e_i\rangle$ have the following inner products $\langle e_i | e_j \rangle = \delta_{ij}$ as they are orthogonal and normalized. Find an expression for $\langle J | I \rangle$ where $|I\rangle = a_i\,|e_1\rangle + b_i\,|e_2\rangle + c_i\,|e_3\rangle$ and $|J\rangle = a_j\,|e_1\rangle + b_j\,|e_2\rangle + c_j\,|e_3\rangle$. Note $\langle J| = a_j^*\,\langle e_1| + b_j^*\,\langle e_2| + c_j^*\,\langle e_3|$ for a complex vector space. See property I3 of the inner product.

b.) Find the component of $|J\rangle$ along $|e_2\rangle$. *What is a component ?* You should create a definition!

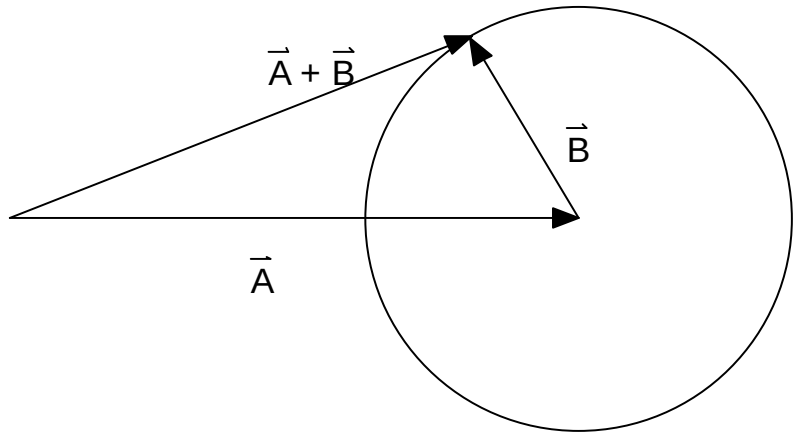
7.) Given any two vectors in an inner product space $|A\rangle$ and $|B\rangle$, prove the Schwarz Inequality: $|\langle A|B\rangle| \le \|A\rangle\|\|B\rangle|$. Use the vector $|C\rangle = |A\rangle - \left[\langle B|B\rangle\right]^{-1}\langle B|A\rangle\,|B\rangle$ and the properties of an inner product. The form of the vector $|C\rangle$ reminds you of a procedure studied in this handout. Name that procedure. Study the dagger operation as it provides the rule for computing the *BRA* vector conjugate to a given *KET* vector. Recall that $|V|^2 = \langle V|V\rangle$.

8.) Argue that $|\langle A|B\rangle + \langle B|A\rangle| \le 2\,|\langle A|B\rangle|$. Hint: Regard $\langle A|B\rangle$ as an arbitrary complex number.

9.) Use the Schwarz Inequality: $|\langle A|B\rangle| \le \|A\rangle\|\|B\rangle|$, the previous problem and $|V|^2 = \langle V|V\rangle$ to establish the triangle inequality: The magnitude of the sum of two vectors is between the magnitude of the difference of the magnitudes of the two vectors and the sum of their magnitudes.

$\big||A\rangle| - |B\rangle\big| \le |\,|A\rangle + |B\rangle\,| \le |A\rangle| + |B\rangle|$ Compare the expressions

$\left|\,|A\rangle|+|B\rangle\,\right|^2 = \langle A|A\rangle + 2\,|A\rangle|\,|B\rangle| + \langle B|B\rangle$ and $\left|\,|A\rangle|-|B\rangle\,\right|^2$ with the expression for $\left|\,|A\rangle+|B\rangle\,\right|^2$.



10.) A vector is expanded in terms of a basis set as $|I\rangle = a\,|e_1\rangle + b\,|e_2\rangle + c\,|e_3\rangle$ where the constants a_i, b_i, and c_i are scalar values. Show that the components of the vector, the values a_i, b_i, and c_i, are unique. HINT: Review the definition of a basis set.

11.) A space of 3rd order polynomials is defined with domain the interval [-1,1]. An inner product for functions on that interval is defined to be:

$$\langle g\,|\,f\rangle = \int_{-1}^{1} g(x)\,f(x)\,dx$$

A possible basis set for the space is { 1, x, x^2, x^3 }. Choose $|B_1\rangle = 1$ and then work upward power by power. Use the Gram-Schmidt process to develop an orthogonal set of vectors (polynomials). Apply the normalization condition the $P_n(1) = 1$ to set the overall scaling (normalization of the polynomials. From Mathematica:

LegendreP[2,x] = $-\frac{1}{2}+\frac{3}{2}\,x^2$; LegendreP[3,x] = $-\frac{3}{2}x+\frac{5}{2}\,x^3$.(See Boas p. 485.)

12.) A space of 3rd order polynomials is defined with domain the interval [-∞,∞]. An inner product for functions on that interval is defined to be:

$$\langle g\,|\,f\rangle = \int_{-\infty}^{\infty} g(x)\,f(x)\;e^{-x^2}\,dx \qquad \text{Note the weight function: } e^{-x^2}$$

A possible basis set for the space is {1, x, x^2, x^3 }. Choose $|B_1\rangle = 1$ and then work upward power by

power. Use the Gram-Schmidt process to develop an orthogonal set of vectors (polynomials). The resulting polynomials are the Hermite polynomials that use yet another weird normalization. For the nth order polynomial, the lead term is $2^n\, x^n$. Multiply the Gram-Schmidt result by whatever factor is necessary to yield the desired highest order term. (See Boas p. 530.)

From Mathematica: HermiteH[2,x] = $4\,x^2 - 2$; HermiteH[3,x] = $8\,x^3 - 12\,x$.

$$\int_{-\infty}^{\infty} x^{2n}\; e^{-x^2}\, dx = \sqrt{\pi}\;\left(n - \tfrac{1}{2}\right)\left(n - \tfrac{3}{2}\right)\ldots\left(\tfrac{1}{2}\right)$$

The integral vanishes for odd powers of x.

13.) An infinite dimensional function space is defined with domain the interval [-∞,∞]. An inner product for functions on that interval is defined to be:

$$\langle g \,|\, f \rangle = \int_{-\infty}^{\infty} g(x)\, f(x)\;\, dx$$

A possible basis set for the space is: $\left\{1\;\, e^{-\left(x^2/2\right)},\; x\;\, e^{-\left(x^2/2\right)},\; x^2\;\, e^{-\left(x^2/2\right)},\; x^3\;\, e^{-\left(x^2/2\right)}, \ldots\right\}$. Choose $\left|B_1\right\rangle = 1\;\, e^{-\left(x^2/2\right)}$ and then work upward using $\left|B_{n+1}\right\rangle = x^n\;\, e^{-\left(x^2/2\right)}$ as an initial basis function. Use the Gram-Schmidt process to develop an orthogonal set of vectors (functions). The resulting functions are the *Hermite functions* and are to be *unity* normalized using the prescribed inner product. Find the first four Hermite functions. (Compare with the harmonic oscillator wave functions found in Harris or Eisberg.) **Hint**: One could just apply the unity normalization to the results of the Hermite polynomial problem above. *What happened to the weight function?*

Use: $\int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi}$ and $\int_{-\infty}^{\infty} x^{2n}\; e^{-x^2}\, dx = \sqrt{\pi}\;\left(n - \tfrac{1}{2}\right)\left(n - \tfrac{3}{2}\right)\ldots\left(\tfrac{1}{2}\right)$

The integral vanishes for odd powers of x.

14.) **a.)** Use the Gram-Schmidt procedure to create an ortho-normal basis from the spanning set $\left\{\hat{i} + \hat{j} + \hat{k};\; \hat{i} - 2\,\hat{j} + \hat{k};\; \hat{k}\right\}$. What is the dimension of the space spanned by the set? Start with $\left|B_1\right\rangle = \hat{i} + \hat{j} + \hat{k}$ and work to the right.

b.) Consider the space spanned by the set of vectors: $\left\{ \hat{i}+\hat{j}+\hat{k}, \hat{i}+\hat{j}, \hat{k} \right\}$. Use the Gram-Schmidt procedure to create an ortho-normal basis for the space. What is the dimension of the space? Start with $\left|B_1\right\rangle = \hat{i}+\hat{j}+\hat{k}$ and work to the right.

c.) Consider the components of each of the vectors in the initial spanning set as the row of a matrix. Compute the determinant of that matrix for the case of exercise one and for the case of exercise two. Comment on the outcomes.

15.) a.) Starting with $\left|B_1\right\rangle$, apply the Gram-Schmidt procedure to develop an ortho-normal basis set from: $\left\{ \left|B_1\right\rangle = \hat{i}+\hat{k};\ \left|B_2\right\rangle = \hat{i}+\hat{j};\ \left|B_3\right\rangle = \hat{k} \right\}$

b.) Compare with the results for the set $\left\{ \left|B_1\right\rangle = \hat{i}+\hat{k};\ \left|B_2\right\rangle = 2\left(\hat{i}+\hat{j}\right);\ \left|B_3\right\rangle = 3\,\hat{k} \right\}$.

c.) Compare with the results for the set $\left\{ \left|B_1\right\rangle = \hat{i}+\hat{j};\ \left|B_2\right\rangle = \hat{i}+\hat{k};\ \left|B_3\right\rangle = \hat{k} \right\}$.

d.) Compare with the results for the set $\left\{ \left|B_1\right\rangle = \hat{i}+\hat{k};\ \left|B_2\right\rangle = \hat{i}+\hat{j};\ \left|B_3\right\rangle = \hat{i} \right\}$.

The Replacement Lemma: Suppose that $\left\{ \left|v_1\right\rangle, \left|v_2\right\rangle, ..., \left|v_m\right\rangle \right\}$ spans a vector space $\mathbb{V}$.

Given any non-zero $\left|w\right\rangle \in \mathbb{V}$, the vector $\left|w\right\rangle$ can be substituted into the spanning set for one of the $\left|v\right\rangle$'s (say $\left|v_i\right\rangle$) and the resulting set $\left\{ \left|w\right\rangle, \left|v_1\right\rangle, \left|v_2\right\rangle, \ldots, \left|v_{i-1}\right\rangle, \left|v_{i+1}\right\rangle, \ldots, \left|v_m\right\rangle \right\}$ still spans the space $\mathbb{V}$.

16.) The set of vectors $\{\hat{i}, \hat{j}, \hat{k}\} = \{\hat{e}_x, \hat{e}_y, \hat{e}_z\}$ is a complete orthonormal basis set for three dimensional vectors such as $\vec{A} = A_x\,\hat{e}_x + A_y\,\hat{e}_y + A_z\,\hat{e}_z$ and $\vec{B} = B_x\,\hat{e}_x + B_y\,\hat{e}_y + B_z\,\hat{e}_z$. Adopt the *new* notation where $\{|1\rangle, |2\rangle, |3\rangle\}$ represents $\{\hat{e}_x, \hat{e}_y, \hat{e}_z\}$ and $\langle A|B\rangle$ represents $\vec{A}\cdot\vec{B}$.

a.) What are $\langle 2|B\rangle$ and $\langle 1|A\rangle$? What are $\langle 1|2\rangle$, $\langle 3|3\rangle$ and $\langle m|n\rangle$?

b.) Evaluate $\sum_{m=1}^{3} \hat{e}_m\ (\hat{e}_m \cdot \vec{A})$ and $\sum_{m=1}^{3} \hat{e}_m\ (\hat{e}_m \cdot \vec{B})$.

c.) Write out $\sum_{m=1}^{3} \hat{e}_m\ (\hat{e}_m \cdot \vec{A})$ in the *new* notation. Repeat for $\sum_{m=1}^{3} \hat{e}_m\ (\hat{e}_m \cdot \vec{B})$.

d.) Consider $\sum_{m=1}^{3}|m\rangle\langle m|$ as an operator on the three dimensional space of vectors. Let $|V\rangle$ be an arbitrary three dimensional vector in this space. What is $\{\sum_{m=1}^{3}|m\rangle\langle m|\}|V\rangle$?

e.) It is said that $\sum_{m=1}^{3}|m\rangle\langle m|$ is equal to 1. What is $1|V\rangle$?

f.) What is $\{\sum_{n=1}^{3}|n\rangle\langle n|\sum_{m=1}^{3}|m\rangle\langle m|\}|\mathrm{V}\rangle$?

g.) Compare $\langle A|B\rangle$ and $\langle A|\{\sum_{n=1}^{3}|n\rangle\langle n|\sum_{m=1}^{3}|m\rangle\langle m|\}|B\rangle = \langle A|\{\sum_{m,n=1}^{3}|n\rangle\langle n|m\rangle\langle m|\}|B\rangle\}$ Evaluate $\langle n|m\rangle$. Execute the sum over *n*. Finally, execute the sum over *m*.

h.) Rewrite $\langle A|\{\sum_{n=1}^{3}|n\rangle\langle n|\sum_{m=1}^{3}|m\rangle\langle m|\}|B\rangle$ using summation convention. That is with summations over repeated indices being implicit removing the need for the Σ's.

i.) Would it make sense to say that $\sum_{m=1}^{3}|m\rangle\langle m|$ is equal to 1? Would it make sense to say that $\sum_{m=1}^{2}|m\rangle\langle m|$ is equal to 1. Why not? The sum should be over the vectors in a complete orthonormal basis set. The operator $\sum_{m=1}^{2}|m\rangle\langle m|$ maps vectors into their projections onto the *x*-*y* (1-2) plane.

17. **The span of a set of vectors**: Consider all the vectors that can be represented as $\sum a_i|I\rangle$ where the a_i are arbitrary scalar coefficients. The set $\mathbb{S}=\{...,|I\rangle,...\}$ is said to ***span*** the space of elements $\sum a_i|I\rangle$.

$$\mathrm{Span}(\{...,|I\rangle,...\})=\{....,\sum a_i|I\rangle,.....\} \text{ for any } \{\ldots a_i\ldots\}\in\mathbb{K}.$$

a.) The members of the set $\mathbb{S}=\{...,|I\rangle,...\}$ are linearly independent. This linearly independence immediately identifies one vector that cannot be a member of the set. What is that excluded vector?

b.) The representation of a vector as a linear combination of vectors in a linearly independent set is unique. Prove this proposition. Begin by assuming that there are two distinct linear combinations of the vectors that equal the vector $|v\rangle$.

$$|v\rangle = a_1|1\rangle + a_2|2\rangle + ... + a_N|N\rangle \text{ and } |v\rangle = b_1|1\rangle + b_2|2\rangle + ... + b_N|N\rangle$$

Show that this assumption leads to a contradiction. It follows immediately that $a_1|1\rangle + a_2|2\rangle + ... + a_N|N\rangle = b_1|1\rangle + b_2|2\rangle + ... + b_N|N\rangle$ requires that $a_i = b_i$ for $1 \le i \le N$. <u>Compare this problem with FS3 and LS9.</u> Add the result from the next problem and compare again!

Consider displacements of lengths 2 meters and 3 meters whose direction make an angle of 75^0 with respect to one another. Are these displacements linearly independent? A third displacement is added to the set. What character must it possess if the set of the three displacements is to be linearly independent?

18.) Consider a set of vectors that is mutually orthogonal. That is: every member has a vanishing inner product with every other member of the set. Prove that the set of vectors is linearly independent. Well, slow down a little. There is one trivial little bothersome vector that can never appear in a set that is to be linearly independent. a.) What is that irksome little vector? b.) Add the statement that the irksome vector is not a member of our set of mutually orthogonal vectors and prove that such a set of mutually orthogonal vectors is linearly independent. The conclusion is that, absent $|\text{zero}\rangle$, a mutually orthogonal set is linearly independent so all propositions proven for linearly independent sets are also true for mutually orthogonal sets. Note that $|\text{zero}\rangle$ cannot be a member of an orthonormal set.

Consider a set of three mutually perpendicular (orthogonal) displacements. Are they linearly independent?

19.) Consider operators defined by their actions on a set of vectors as:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \text{ and } \hat{b}|n\rangle = \sqrt{n+1}|n+1\rangle \text{ where } \langle m|n\rangle = \delta_{mn}$$

The vector labels are the real positive integers: ($0 \le n < \infty$). Show that $\langle \hat{b}\, m|n\rangle = \langle m|\hat{a}\, n\rangle = \langle m|(\hat{a}|n\rangle)$ for all m and n. Note that you must get must get the operator to the KET side to use its defined operation. Use inner product property I3:

$\left\langle \hat{b}\, m \middle| n \right\rangle = \left\langle n \middle| \hat{b}\, m \right\rangle^* = \left[\langle n | \left(\hat{b} | m \rangle \right) \right]^*$. This final result suggests that there might be a special relationship between the operators $\hat{a}$ and $\hat{b}$. What is that relationship?

20.) Consider the vector space $\mathbb{V}$ containing all the vectors that are linear combinations of the orthonormal basis set $\{|0\rangle, |1\rangle, |2\rangle, ..., ...\}$ introduced in the previous problem. (READ the previous problem before proceeding. The task is to be repeated the previous problem for $\hat{b}$ and $\hat{a}$ acting on general vectors rather than just on basis vectors. Note that even the most general vector can be represented as a linear combination of the basis vectors.)

General Vectors: $|\psi\rangle = \sum_{n=0}^{\infty} c_{\psi n} |n\rangle \qquad \langle \psi | = \sum_{k=0}^{\infty} c_{\psi k}^* \langle k | \qquad |\phi\rangle = \sum_{m=0}^{\infty} c_{\phi m} |m\rangle$

The operators defined by their actions on a set of *basis* vectors as:

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \text{ and } \hat{b}|n\rangle = \sqrt{n+1}\,|n+1\rangle \text{ where } \langle m|n\rangle = \delta_{mn}$$

It follows from the previous problem that $\left\langle \hat{b}\, m \middle| n \right\rangle = \langle m | \hat{a}\, n \rangle = \langle m | \left(\hat{a} | n \rangle \right)$ for all m and n.

Show that, in general, $\langle \psi | \hat{a} | \phi \rangle = \langle \psi | \hat{a}\, \phi \rangle = \left\langle \hat{b}\, \psi \middle| \phi \right\rangle$ for all $|\psi\rangle$ and $|\phi\rangle$ in the space. This result firmly establishes that $\hat{b} = (\hat{a})^\dagger$.

It must be shown that $\langle \psi | \hat{a}\, \phi \rangle = \left\langle \hat{b}\, \psi \middle| \phi \right\rangle$ for all vectors $|\phi\rangle$ and $|\psi\rangle \in \mathbb{V}$ to show that $\hat{b} = (\hat{a})^\dagger$. We conclude that it is only necessary to verify the adjoint property of a linear operator for all the vectors in a basis. It then follows for all vectors in the space using linearity and the fact that any vector in the space is a linear combination of basis vector.

In as much as the operators are linear, the result in the previous problem that $\left\langle \hat{b}\, m \middle| n \right\rangle = \langle m | \hat{a}\, n \rangle$ for all $|m\rangle$ and $|n\rangle$ in the basis set ensures that: $\langle \psi | \hat{a}\, \phi \rangle = \left\langle \hat{b}\, \psi \middle| \phi \right\rangle$.

21.) Consider the bizarre operators defined by their actions as: $(0 \le n < \infty)$

$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$ and $\hat{a}^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$. Sketch the forms of the matrices for these operators. The

state vectors satisfy the ortho-normality condition $\langle n|m\rangle = \delta_{mn}$. Each matrix entry $[\,\hat{a}\,]_{mn}$ is $\langle m|\hat{a}|n\rangle = \langle m|\hat{a}\,n\rangle$. By repeating the operations, it follows that: $\hat{a}^2|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle$; $\hat{a}^\dagger\,\hat{a}|n\rangle = n|n\rangle$ and $\left(\hat{a}^\dagger\right)^2|n\rangle = \sqrt{(n+1)(n+2)}\,|n+2\rangle$. What is $\hat{a}\,\hat{a}^\dagger|n\rangle$? What is $(\hat{a}\,\hat{a}^\dagger - \hat{a}^\dagger\hat{a})|n\rangle$?

22.) Sketch the forms of the matrices for the operators: $\hat{a}^2$; $\hat{a}^\dagger\,\hat{a}$ and $\left(\hat{a}^\dagger\right)^2$. Show that these results can be found as corresponding matrix products of the matrices for the individual operators $\hat{a}$ and $\hat{a}^\dagger$.

22.1) The quantum oscillator state $|\,k\rangle$ is represented by the column vector with zeroes everywhere except in row $k + 1$. (Recall that the QHO representation starts at $n = 0$.) Form the column vector (*the first six rows*) that represents the state $|2\rangle$. Matrix multiply on the left by the matrices representing $\hat{a}^2$; $\hat{a}^\dagger\,\hat{a}$ and $\left(\hat{a}^\dagger\right)^2$. Identify the result of the multiplication in each case.

22.2) The quantum oscillator state $|\,k\rangle$ is represented by the column vector with zeroes everywhere except in row $k + 1$. (Recall that the QHO representation starts at $n = 0$.) Form the column vector (*the first six rows*) that represents $\frac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right]$. The hamiltonian is $½\hbar\omega_0\left[\hat{a}^\dagger\,\hat{a} + \hat{a}\,\hat{a}^\dagger\right]$ and $\left[\hat{a}^\dagger\,\hat{a} + \hat{a}\,\hat{a}^\dagger\right]$ has a matrix representation that is diagonal with diagonal values $2\,n + 1$. That is: the element in (row 0, column 0) is 1. The matrix representation for the state bra is the Hermitian conjugate (complex conjugate of the transpose, a row vector). Display it. Use the matrices to compute $\frac{1}{\sqrt{2}}\left[\langle 1| - \langle 3|\right] | \frac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right]$, the normalization inner product, and $\frac{1}{\sqrt{2}}\left[\langle 1| - \langle 3|\right]\hat{H} \,|\, \frac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right]$, the expectation value of the energy in the state. For $\frac{1}{\sqrt{2}}\left[\langle 1| - \langle 3|\right]\hat{H} \,|\, \frac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right]$, $\frac{1}{\sqrt{2}}\left[|1\rangle - |3\rangle\right]$ is a column vector which is multiplied by the matrix that represents $\hat{H}$ which, in turn, is multiplied on the left by the row matrix that represents the bra, $\frac{1}{\sqrt{2}}\left[\langle 1| - \langle 3|\right]$. Repeat the calculations for the general state $|\psi\rangle = \sum_{k=0}^{\infty} a_k\,|k\rangle$ so that the matrix representing $|\psi\rangle$ is the column matrix of the a_k's . What interpretation do you assign to the value $a_m{}^*\,a_m$?

23.) It is proposed that the inner product of complex-valued functions with the domain of the real line (∞, - ∞) be defined as: $\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} [\phi(x)]^* \psi(x)\, dx$. The operation returns a scalar value as required. Show that the proposed definition meets the requirements of the four axioms for inner products. The space of function is restricted to functions ζ(*x*) such that $\int_{-\infty}^{\infty} |\zeta(x)|^2\, dx$ is defined ⇒ that is: functions that are square integrable.

24.) Suppose that $\langle \phi | \psi \rangle = \int_{-\infty}^{\infty} [\phi(x)]^* \psi(x)\, dx$ is a valid inner product for complex-valued functions with the domain of the real line (∞, - ∞). What can be said about the values ⟨ϕ|ψ⟩, ⟨ψ|ψ⟩ and ⟨ϕ|ϕ⟩? What name is associated with the relationship that you propose?

25.) Show that ⟨V|**ZERO** ⟩ = 0 for all vectors |V ⟩. Build your proof on the properties of the inner product.

26.) Suppose that |*n*⟩ is represented by a column vector with zeros in each row except for row *n* which has a one. (Recall: rows are numbered 0, 1, 2, … .) Multiply a column matrix for the state *n* on the left by matrices $\underset{\approx}{\hat{a}}$ and $\underset{\approx}{\hat{a}}^{\dagger}$ that represent $\hat{a}$ and $\hat{a}^{\dagger}$. Do the matrices provide a *faithful*, working representation of the operators and states? Let them operate (*multiply*) the column vector for the state |3⟩. What matrix representation would you choose for ⟨*m*|? … for the inner product ⟨*m*|*n*⟩? Do your results support the claim that the matrix representing an operator is the complex conjugate of the transpose of the matrix representing the adjoint operator? Start by examining the matrices $\underset{\approx}{\hat{a}}$ and $\underset{\approx}{\hat{a}}^{\dagger}$ for $\hat{a}$ and $\hat{a}^{\dagger}$. In *matrix-speak*, the complex conjugate of the transpose is called the Hermitian conjugate.

27.) Show that for two operators $\hat{O}_1$ and $\hat{O}_2$ that $\left[\hat{O}_1\ \hat{O}_2\right]^{\dagger} = \hat{O}_2^{\dagger}\hat{O}_1^{\dagger}$. The Hermitian conjugate of a product of operators is the product of the Hermitian conjugates of the individual operators taken in the ***reverse order***.

Compare with the results for matrices that: $(\mathbb{A}\,\mathbb{B})^t = \mathbb{B}^t\,\mathbb{A}^t$ and $(\mathbb{A}\,\mathbb{B})^{-1} = f\,\mathbb{B}^{-1}\,\mathbb{A}^{-1}$

28.) Given an operator $\hat{O}$ and its Hermitian conjugate $\hat{O}^{\dagger}$, show that the operators $\hat{S} = ½[\hat{O} + \hat{O}^{\dagger}]$ and $\hat{A} = \frac{i}{2}[\hat{O} - \hat{O}^{\dagger}]$ are Hermitian. Note that the defining property for the conjugate or adjoint operator involves replacing an action on the KET by an action on the BRA. Which of the inner product axioms involves interchanging BRAs and KETs?

29.) Once a basis set has been identified for a vector space $\mathbb{V}$, operators on that space can be represented by matrices that reference that basis set. Suppose the basis set $\mathbb{S}$ is { … , $|n\rangle$, … , $|m\rangle$, … }. The matrix that represents the operator $\hat{O}$ has elements $\left[\underset{\approx}{0}\right]_{mn} = \langle m|\hat{O}|n\rangle$. Find the relation that defines the adjoint operator $\hat{O}^{\dagger}$ and copy it as an initial step. Use this relation and the properties of the inner product to show that $\langle m|\hat{O}|n\rangle = \langle m|(\hat{O}|n\rangle)$ and $\langle \hat{O}^{\dagger}m|\, n\rangle = \langle n||\hat{O}^{\dagger}m\rangle^{*}$. That is: $\left[\underset{\approx}{0}\right]_{mn} = \left(\left[\underset{\approx}{0}^{\dagger}\right]_{nm}\right)^{*}$. Use this to show that the matrix that represents a Hermitian operator is equal to the complex conjugate of its transpose. The complex conjugate of the transpose of a matrix is called its Hermitian conjugate. The symbol $\underset{\approx}{0}$ is the *rectangular array of numbers* that represent the operator $\hat{O}$ given the choice of basis $\mathbb{S}$. (The exact values in that array depend on the choice of basis just as the three components of the gravitational, the *linear array of three numbers representing* $\vec{g}$, field depend on the choice of the basis vectors $\Rightarrow$ the orientation of the axes. This issue is tackled in the linear transformations handout.)

Quantum Problems:

1. Prove that eigenvalues of Hermitian operators are real.
2. Prove that eigenvectors of a Hermitian operator with distinctly different eigenvalues are orthogonal.
3. Starting from the energy eigenvalue equation H |Ψ> = E | Ψ >, show that by expanding in a complete set of states |j> that this becomes the matrix equation

$$\sum_j \langle i|H|j\rangle\langle j|\Psi\rangle \quad = \quad E_i \langle i|\Psi\rangle$$

4. Show that the commutator $[x, p_x] = i\hbar$

5. Show that the commutator $[V, p_x] = i\hbar \dfrac{dV}{dx}$

6. Starting from the basic equation which gives the time evolution of expectation values, show that $\dfrac{d}{dt}\langle p \rangle = -\langle \nabla V \rangle$, which can be interpreted as the equivalent Newton's Equation of Motion $^{dp}/_{dt}$ = F from kindergarten physics. $\dfrac{d}{dt}\langle A \rangle = \dfrac{1}{i\hbar}\langle [A, H] \rangle + \left\langle \dfrac{\partial A}{\partial t} \right\rangle$

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