Lecture 7

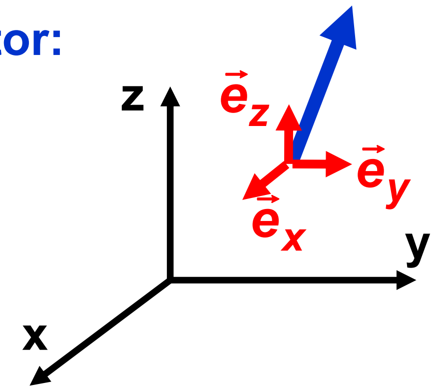
A Math Primer for Quantum Physics

In this lecture you will learn:

- **Vector spaces and Hilbert spaces**
- **Operators in Hilbert spaces**
- **Basis sets**

Lessons from Electromagnetism: Basis and Representation

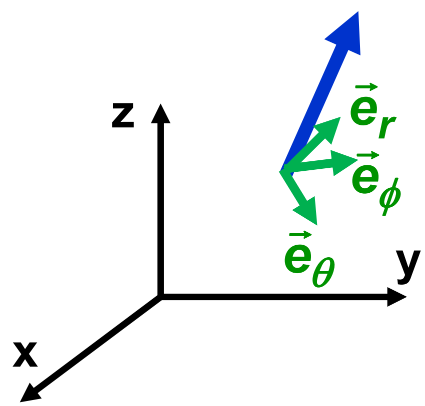
Consider an electric field vector:



$$\vec{E} = E_x\vec{e}_x + E_y\vec{e}_y + E_z\vec{e}_z$$

Now change the representation basis :

$$\vec{E} = E_x\vec{e}_x + E_y\vec{e}_y + E_z\vec{e}_z$$
$$= E_r\vec{e}_r + E_\phi\vec{e}_\phi + E_\theta\vec{e}_\theta$$



The same vector can be represented in different ways using different unit vector basis sets for its representation

Lessons from Electromagnetism: Physics in Basis-Independent Representation

(1) $\nabla . \varepsilon_o \vec{E} = \rho$ Gauss' Law

(2) $\nabla . \mu_o \vec{H} = 0$ Gauss' Law

(3) $\nabla \times \vec{E} = -\frac{\partial \mu_o \vec{H}}{\partial t}$ Faraday's Law

(4) $\nabla \times \vec{H} = \vec{J} + \frac{\partial \varepsilon_o \vec{E}}{\partial t}$ Ampere's Law

James Clerk Maxwell
(1831-1879)

It is better to do physics in a representation-independent way!!

The Quantum State

A quantum state (of any particle or system) is represented by the state vector $|\psi(t)\rangle$ which is a vector in a Hilbert space

Vector Spaces and Hilbert Spaces

Vectors (or kets) of dimension *N* are said to form a Hilbert space $\mathbb{H}$ or belong to a Hilbert space $\mathbb{H}$ if:

1) **For any two vectors** $|v\rangle \in \mathbb{H}$ **and** $|u\rangle \in \mathbb{H}$, $|v\rangle + |u\rangle = |u\rangle + |v\rangle \in \mathbb{H}$

2) $|v\rangle + 0 = 0 + |v\rangle = |v\rangle$

3) **For any vector** $|v\rangle \in \mathbb{H}$, $\alpha|v\rangle \in \mathbb{H}$ (α **is any complex number)**

4) **For any two vectors** $|v\rangle \in \mathbb{H}$ **and** $|u\rangle \in \mathbb{H}$, $\alpha(|v\rangle + |u\rangle) = \alpha|v\rangle + \alpha|u\rangle)$

Examples of vectors (or kets): column vectors

$$|v\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \qquad |v\rangle = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

Vector Spaces and Hilbert Spaces

Dual vectors (or bras) are defined as:

$$|v\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \iff \langle v| = \begin{bmatrix} a^* & b^* \end{bmatrix}$$

Vector (or ket) Dual vector (or bra)

$$\alpha|v\rangle = \alpha\begin{bmatrix} a \\ b \end{bmatrix} \iff \alpha^*\langle v| = \alpha^*\begin{bmatrix} a^* & b^* \end{bmatrix}$$

Vector (or ket) Dual vector (or bra)

Dual vectors (or bras) also form a Hilbert space of their own!

Inner Product and Norm

An inner product is defined between a vector (ket) and a dual vector (bra) as follows:

Given two vectors $|\mathrm{v}\rangle$ and $|\mathrm{u}\rangle$ belonging to a $\mathbb{H}$:

$$|v\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \qquad |u\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$$

The inner product between these two vectors is defined as:

$$\langle u|v\rangle = \left(\langle v|u\rangle\right)^* = \begin{bmatrix} c^* & d^* \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = c^*a + d^*b$$

Two different vectors are said to be orthogonal if there inner product is zero

The norm of a vector is defined as follows and is always non-negative and real:

$$\left\| |v\rangle \right\|^2 = \langle v|v\rangle = \begin{bmatrix} a^* & b^* \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = |a|^2 + |b|^2 \geq 0$$

Operators

An operator $\hat{O}$ acting in a Hilbert space has the property that it takes a vector in the Hilbert space to some other vector in the same Hilbert space

For a vector $|v\rangle \in \mathbb{H}$, the action of the operator gives another vector $|u\rangle \in \mathbb{H}$,

$$|u\rangle = \hat{O}|v\rangle$$

Example: Operators are represented by matrices in the Hilbert space of column vectors

$$\hat{O} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad |v\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$|u\rangle = \hat{O}|v\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} b \\ a \end{bmatrix}$$

Exterior Product

An exterior product between a vector (ket) and a dual vector (bra) is defined as follows:

Given two vectors $|\mathrm{v}\rangle$ and $|\mathrm{u}\rangle$:

$$|v\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \qquad |u\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$$

The exterior product between these two vectors is an operator:

$$|v\rangle\langle u| = \begin{bmatrix} a \\ b \end{bmatrix}\begin{bmatrix} c^* & d^* \end{bmatrix} = \begin{bmatrix} ac^* & ad^* \\ bc^* & bd^* \end{bmatrix}$$

To see why it is an operator, take a third vector $|\mathrm{w}\rangle$ and act upon it with the exterior product:

$$\big(|v\rangle\langle u|\big)|w\rangle = |v\rangle\langle u|w\rangle = \langle u|w\rangle|v\rangle$$

Another vector

Adjoint Operators

Adjoint Operator: **Suppose $\hat{O}$ is an operator then the adjoint of $\hat{O}$, indicated as $\hat{O}^\dagger$, is defined by the equation:**

$$\langle v|\hat{O}|u\rangle = \left(\langle u|\hat{O}^\dagger|v\rangle\right)^*$$

Suppose we define a new vector $|w\rangle$ as:

$$|w\rangle = \hat{O}|u\rangle$$

This implies:

$$\langle v|w\rangle = \langle v|\hat{O}|u\rangle = \left(\langle w|v\rangle\right)^* = \left(\langle u|\hat{O}^\dagger|v\rangle\right)^*$$

Therefore the dual vector corresponding to $|w\rangle$ must obey:

$$|w\rangle = \hat{O}|u\rangle \longrightarrow \langle w| = \langle u|\hat{O}^\dagger$$

Adjoint Operators

Example:

$$\hat{O} = \begin{bmatrix} 0 & i \\ 1 & 0 \end{bmatrix} \qquad |u\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$|w\rangle = \hat{O}|u\rangle = \begin{bmatrix} 0 & i \\ 1 & 0 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} ib \\ a \end{bmatrix}$$

Which gives:

$$\langle w| = \begin{bmatrix} -ib^* & a^* \end{bmatrix} = \begin{bmatrix} a^* & b^* \end{bmatrix}\begin{bmatrix} 0 & 1 \\ -i & 0 \end{bmatrix} = \langle u|\hat{O}^\dagger$$

This means that the adjoint operator is just the Hermitian conjugate matrix:

$$\hat{O}^\dagger = \begin{bmatrix} 0 & 1 \\ -i & 0 \end{bmatrix}$$

Self-Adjoint Operators or Hermitian Operators

An operator is called self-adjoint or Hermitian if it equals its adjoint:

$$\hat{O} = \hat{O}^{\dagger}$$

Example:

$$\hat{O} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \hat{O}^{\dagger}$$

Eigenvalues and Eigenvectors of Operators

Suppose $\hat{O}$ is an operator then the eigenvectors and eigenvalues of this operator are defined by the equation:

$$\hat{O}\left|v\right\rangle = \lambda\left|v\right\rangle$$

Eigenvector ($\left|v\right\rangle$), Eigenvalue (λ)

An operator can have a large number of eigenvectors and eigenvalues:

$$\hat{O}\left|v_j\right\rangle = \lambda_j\left|v_j\right\rangle \qquad \{ j = 1, 2, 3.....$$

Example:

$$\hat{O} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\lambda_1 = +1 \qquad \left|v_1\right\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

$$\lambda_2 = -1 \qquad \left|v_2\right\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

Eigenvectors and Eigenvalues: Hermitian Operators

1) A Hermitian operator (or a self-adjoint matrix) has real eigenvalues:

Proof:

$$\hat{O}|v\rangle = \lambda |v\rangle$$

$$\Rightarrow \langle v|\hat{O}^\dagger = \lambda^* \langle v|$$

$$\Rightarrow \langle v|\hat{O}^\dagger|v\rangle = \lambda^* \langle v|v\rangle$$

$$\Rightarrow \langle v|\hat{O}|v\rangle = \lambda^* \langle v|v\rangle$$

$$\Rightarrow \lambda \langle v|v\rangle = \lambda^* \langle v|v\rangle$$

$$\Rightarrow \lambda = \lambda^*$$

Eigenvectors and Eigenvalues: Hermitian Operators

2) Different eigenvectors of a Hermitian operator are orthogonal

Proof:

Suppose: $\hat{O}\left|v_1\right\rangle = \lambda_1\left|v_1\right\rangle \qquad \hat{O}\left|v_2\right\rangle = \lambda_2\left|v_2\right\rangle$

$$\hat{O}\left|v_1\right\rangle = \lambda_1\left|v_1\right\rangle$$

$$\Rightarrow \left\langle v_2\middle|\hat{O}\middle|v_1\right\rangle = \lambda_1\left\langle v_2\middle|v_1\right\rangle$$

$$\Rightarrow \left(\left\langle v_1\middle|\hat{O}^\dagger\middle|v_2\right\rangle\right)^* = \lambda_1\left\langle v_2\middle|v_1\right\rangle$$

$$\Rightarrow \left(\left\langle v_1\middle|\hat{O}\middle|v_2\right\rangle\right)^* = \lambda_1\left\langle v_2\middle|v_1\right\rangle$$

$$\Rightarrow \left(\lambda_2\left\langle v_1\middle|v_2\right\rangle\right)^* = \lambda_1\left\langle v_2\middle|v_1\right\rangle$$

$$\Rightarrow \lambda_2\left\langle v_2\middle|v_1\right\rangle = \lambda_1\left\langle v_2\middle|v_1\right\rangle$$

$$\Rightarrow (\lambda_2 - \lambda_1)\left\langle v_2\middle|v_1\right\rangle = 0$$

→ If $\lambda_1 \neq \lambda_2$ then the eigenvectors are orthogonal

What we just showed is that eigenvectors corresponding to *different* eigenvalues are orthogonal

What if $\lambda_1 = \lambda_2$?

In that case, it can be shown that the two eigenvectors v_1 and v_2 can be chosen to be orthogonal

Eigenvectors and Eigenvalues: Hermitian Operators

Example:

$$\hat{O} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\lambda_1 = +1 \qquad |v_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

$$\lambda_2 = -1 \qquad |v_2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

$$\Longrightarrow \quad \langle v_2 | v_1 \rangle = 0$$

Unity Operator

A unity operator, indicated by $\hat{1}$, acting upon a vector gives back the same vector:

$$\hat{1}|v\rangle = |v\rangle$$

Example:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a \\ b \end{bmatrix}$$

Identity matrix

Complete Basis Set

A set of vectors are said to span a Hilbert space and form a complete basis set if any arbitrary vector in the Hilbert space can be expressed as a linear combination (or as a superposition) of the vectors in this basis set

If the vectors $|v_j\rangle \quad (j = 1, 2, 3.....N)$ form a complete set then for any vector $|u\rangle$:

$$|u\rangle = \sum_{j=1}^{N} a_j |v_j\rangle$$

The smallest number of vectors needed in a complete basis set to span a Hilbert space is called the dimension of the Hilbert space

Complete Basis Set

Example:

Consider the two-dimensional Hilbert space of column vectors and suppose:

$$|v_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |v_2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

You can convince yourself that any vector $\begin{bmatrix} a \\ b \end{bmatrix}$ **can be written as:**

$$\begin{bmatrix} a \\ b \end{bmatrix} = a|v_1\rangle + b|v_2\rangle$$

Therefore, the dimensionality of the Hilbert space is 2

Orthonormal Basis Set

If all the vectors in a basis set are orthogonal to each other and are normalized to unity, then they are said to constitute an orthonormal basis set

If the vectors $|v_j\rangle \quad (j = 1,2,3.....N)$ **form an orthonormal basis set then:**

$$\langle v_k | v_j \rangle = \delta_{kj} \qquad \text{and} \qquad \sum_{j=1}^{N} |v_j\rangle\langle v_j| = \hat{1} = \text{unity operator}$$

Any arbitrary vector $|u\rangle$ **can be expanded as a linear superposition of the vectors in an orthonormal basis set:**

$$|u\rangle = \sum_j \alpha_j v_j$$

Multiply both sides by $\langle v_k|$ **:**

$$\langle v_k | u \rangle = \sum_j \alpha_j \langle v_k | v_j \rangle$$

$$\Rightarrow \langle v_k | u \rangle = \sum_j \alpha_j \, \delta_{kj}$$

$$\Rightarrow \langle v_k | u \rangle = \alpha_k$$

$$\Rightarrow \alpha_k = \langle v_k | u \rangle$$

Alternatively, we can write:

$$|u\rangle = \hat{1}|u\rangle$$

$$= \left(\sum_{j=1}^{N} |v_j\rangle\langle v_j| \right)|u\rangle$$

$$= \sum_{j=1}^{N} |v_j\rangle\langle v_j | u\rangle$$

$$= \sum_j \alpha_j v_j \longrightarrow \alpha_j = \langle v_j | u \rangle$$

Expansion coefficients

Orthonormal Basis Set

Example:

Consider the two-dimensional Hilbert space of column vectors with the following orthonormal complete basis set:

$$|v_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad |v_2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Then:

$$\sum_{j=1}^{2} |v_j\rangle\langle v_j| = \hat{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Eigenvectors and Eigenvalues: Hermitian Operators

Normalized (to unity) eigenvectors of any Hermitian operator form an orthonormal complete basis set

Example:

$$\hat{O} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\lambda_1 = +1 \qquad |v_1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

$$\lambda_2 = -1 \qquad |v_2\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

$$\Rightarrow \quad \sum_{j=1}^{2} |v_j\rangle\langle v_j| = \hat{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Matrix Representation of an Operator

Consider an operator $\hat{O}$ belonging to some abstract Hilbert space

And suppose we have a complete basis set in that Hilbert space:

$$\sum_{j} |v_j\rangle\langle v_j| = \hat{1} = \text{unity operator}$$

We can write the operator as:

$$\hat{O} = \hat{1}\,\hat{O}\,\hat{1} = \left(\sum_{j} |v_j\rangle\langle v_j|\right)\hat{O}\left(\sum_{m} |v_m\rangle\langle v_m|\right)$$

$$= \sum_{j,m} \langle v_j|\hat{O}|v_m\rangle\ |v_j\rangle\langle v_m| = \sum_{j,m} O_{jm}\ |v_j\rangle\langle v_m|$$

An operator is completely defined by these numbers

If two Hilbert spaces have the same dimensionality then one can be chosen to represent the other

Matrix Representation of an Operator

Can we represent an operator, acting in some abstract Hilbert space of dimension *N*, using *N*x*N* matrices and the Hilbert space of column vectors of size *N*? And, if so, how?

Start from:

$$\hat{O} = \hat{1}\,\hat{O}\,\hat{1} = \left(\sum_{j} |v_j\rangle\langle v_j| \right) \hat{O} \left(\sum_{m} |v_m\rangle\langle v_m| \right)$$

$$= \sum_{j,m} \langle v_j|\hat{O}|v_m\rangle \; |v_j\rangle\langle v_m| = \sum_{j,m} O_{jm} \; |v_j\rangle\langle v_m|$$

An operator is completely defined by these numbers

Then make the mapping from the abstract Hilbert space to the Hilbert space of column vectors:

$$|v_1\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \\ . \\ . \\ 0 \end{bmatrix} \qquad |v_2\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \\ 0 \\ . \\ . \\ 0 \end{bmatrix} \qquad |v_3\rangle \rightarrow \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ . \\ 0 \end{bmatrix} \quad \ldots\ldots\ldots$$

In this chosen column vector Hilbert space, the operator is the following *N*x*N* matrix:

$$\hat{O} \rightarrow \begin{bmatrix} . & . & . & . & . & . \\ . & . & O_{(j-1)m} & . & . & . \\ . & O_{j(m-1)} & O_{jm} & O_{j(m+1)} & . & . \\ . & . & O_{(j+1)m} & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{bmatrix}$$

Operator Representation: Switching Basis

Consider the operator in the representation defined by the basis $|v_1\rangle$ and $|v_2\rangle$:

$$|v_1\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |v_2\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \Rightarrow \quad \hat{O} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

The operator has the following eigenvalues and eigenvectors:

$$\lambda_1 = +1 \Rightarrow |e_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \qquad \lambda_2 = -1 \Rightarrow |e_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -i \end{bmatrix}$$

Suppose we want to switch the representation to the basis $|e_1\rangle$ and $|e_2\rangle$:

$$\hat{O} = \hat{1}\,\hat{O}\,\hat{1} = \left(\sum_{j=1}^{2} |e_j\rangle\langle e_j| \right) \hat{O} \left(\sum_{m=1}^{2} |e_m\rangle\langle e_m| \right)$$

$$= \sum_{j,m} \langle e_j|\hat{O}|e_m\rangle \; |e_j\rangle\langle e_m| = \lambda_1 \; |e_1\rangle\langle e_1| + \lambda_2 \; |e_2\rangle\langle e_2|$$

Therefore in the new representation:

$$|e_1\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |e_2\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \Rightarrow \quad \hat{O} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} = \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}$$

Operator is always diagonal in the representation of its eigenvectors!!

Commutation Relations

Operator multiplication (like matrix multiplication) generally depends on the order of multiplication

The way to express this fact is using the commutator:

$$\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Example:

$$\hat{A} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{B} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\left[\hat{A},\hat{B}\right] = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = 2i\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Commutating Operators and Common Set of Eigenvectors

If two operators commute then they both can have the same eigenvectors

Proof:

Suppose: $\left[\hat{A},\hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0$

And suppose $\hat{B}$ has the eigenvectors given by: $\hat{B}\left|v_j\right\rangle = \lambda_j\left|v_j\right\rangle$

Then we need to show that $\left|v_j\right\rangle$ are also the eigenvectors of the operator $\hat{A}$, i.e. $\hat{A}\left|v_j\right\rangle = \gamma_j\left|v_j\right\rangle$

$$\hat{A}\hat{B} - \hat{B}\hat{A} = 0$$

$$\Rightarrow \hat{A}\hat{B}\left|v_j\right\rangle - \hat{B}\hat{A}\left|v_j\right\rangle = 0$$

$$\Rightarrow \hat{A}\lambda_j\left|v_j\right\rangle = \hat{B}\hat{A}\left|v_j\right\rangle$$

$$\Rightarrow \hat{B}\left(\hat{A}\left|v_j\right\rangle\right) = \lambda_j\left(\hat{A}\left|v_j\right\rangle\right)$$

The above can be true if $\hat{A}\left|v_j\right\rangle \propto \left|v_j\right\rangle$ and therefore $\left|v_j\right\rangle$ is also an eigenvector of $\hat{A}$

(Proof is a bit more complicated if the operator $\hat{B}$ has a degenerate eigensubspace)

Hilbert Space of Square Integrable Functions with Zero BC

This space contains all functions *f*(*x*), defined over a space interval *L*, that obey:

$$\int_0^L dx\,\left|f(x)\right|^2 < \infty \qquad \text{and} \qquad f(x) \rightarrow 0 \;\text{ as }\; x \rightarrow 0, L$$

Inner product between two different vectors is defined as:

$$\int_0^L dx\; g^*(x)\, f(x)$$

Vector norm is defined as:

$$\int_0^L dx\,\left|f(x)\right|^2$$

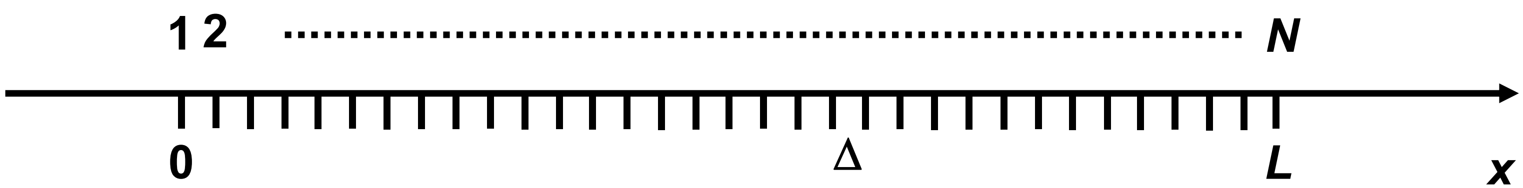
The dimension of this Hilbert space is infinite!

Any linear differential operator would be an example of an operator acting in this Hilbert space:

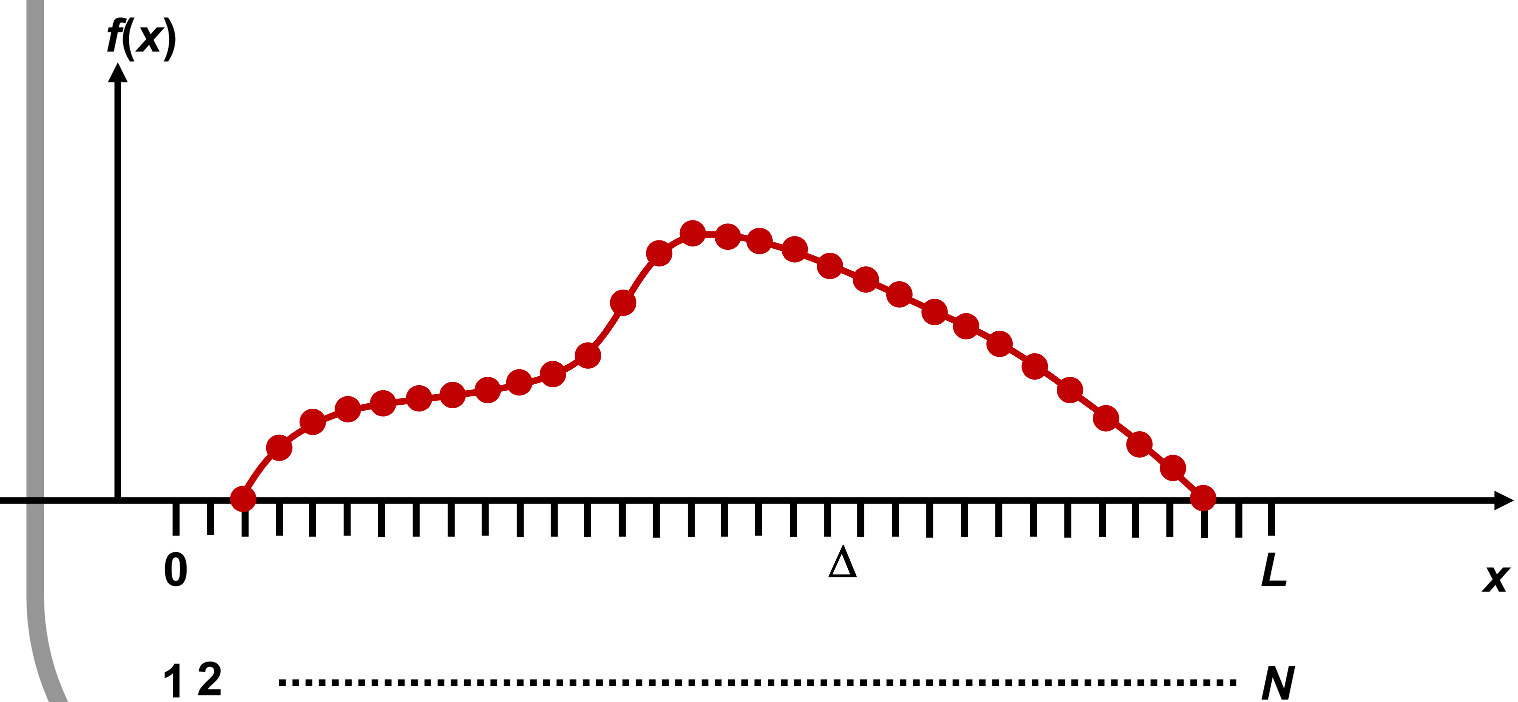
Example: $$g(x) = \hat{O} f(x) = \left[a(x)\frac{\partial^2}{\partial x^2} + b(x)\frac{\partial}{\partial x} + c(x) \right] f(x)$$

Column Vector Representation of the Hilbert Space of Square Integrable Functions

Suppose we divide the space of length L into N intervals of size Δ :



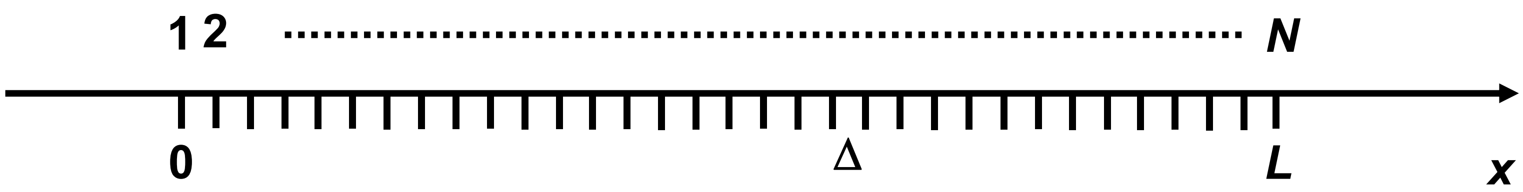
And we approximately represent every vector $f(x)$ by its N values, $f_j = f\left(x_j\right)$, as a column vector in a N-dimensional Hilbert space:



$f(x)$ ⇩

$$\left| f \right\rangle = \begin{bmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ \\ f_N \end{bmatrix} \begin{matrix} 1 \\ 2 \\ \\ \\ \\ \\ \text{N} \end{matrix}$$

Column Vector Representation of the Hilbert Space of Square Integrable Functions



$f(x)$ ⇩

$$|f\rangle = \begin{bmatrix} f_1 \\ f_2 \\ . \\ . \\ . \\ \\ f_N \end{bmatrix} \begin{matrix} 1 \\ 2 \\ \\ \\ \\ \\ N \end{matrix}$$

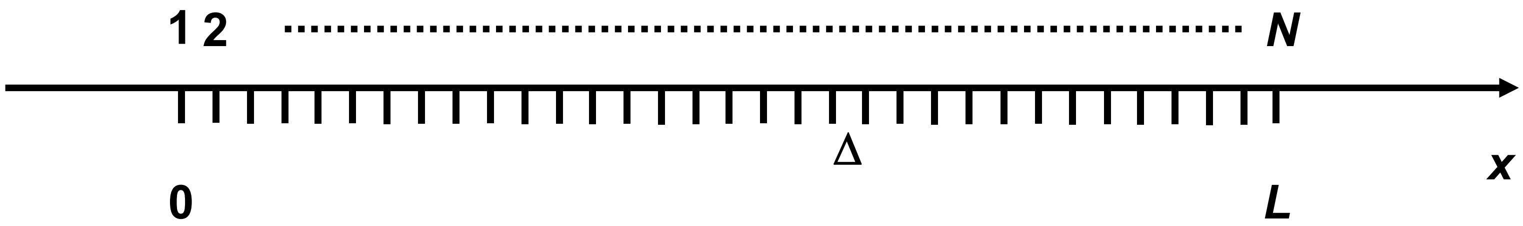
$g(x)$ ⇩

$$|g\rangle = \begin{bmatrix} g_1 \\ g_2 \\ . \\ . \\ . \\ \\ g_2 \end{bmatrix}$$

If N is sufficiently large, one can represent any function over the interval 0 to L by these column vectors or kets in a N-dimensional Hilbert space

We will take the limit $\Delta \rightarrow 0$, or $N \rightarrow \infty$, in the end

Inner Product and Norm



Hilbert spaces require a well-defined inner-product

$f(x)$ ⇓

$$|f\rangle = \begin{bmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ \\ f_N \end{bmatrix} \begin{matrix} 1 \\ 2 \\ \\ \\ \\ \\ N \end{matrix}$$

$g(x)$ ⇓

$$|g\rangle = \begin{bmatrix} g_1 \\ g_2 \\ \cdot \\ \cdot \\ \cdot \\ \\ g_2 \end{bmatrix}$$

Inner Product:

Note this ↓

$$\langle g|f\rangle = \left(g_1^* f_1 + g_2^* f_1 + \ldots\ldots + g_N^* f_N\right)\Delta$$

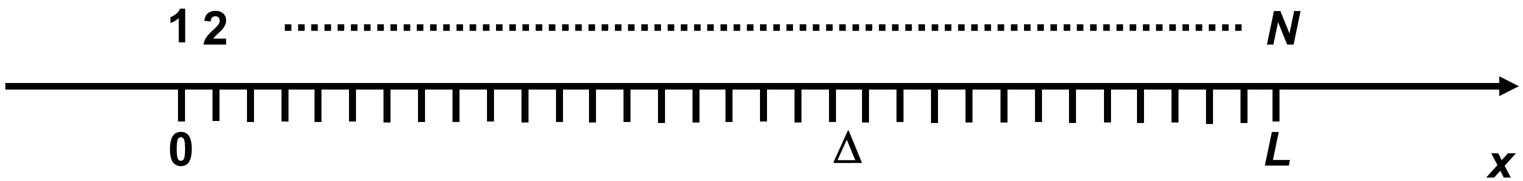
$$\xrightarrow{Lt\ \Delta\to 0} \approx \int_0^L dx\ g^*(x)\, f(x)$$

Vector Norm:

$$\big\||f\rangle\big\|^2 = \langle f|f\rangle = \int_0^L dx\ f^*(x)\, f(x)$$

$$= \int_0^L dx\ |f(x)|^2 < \infty$$

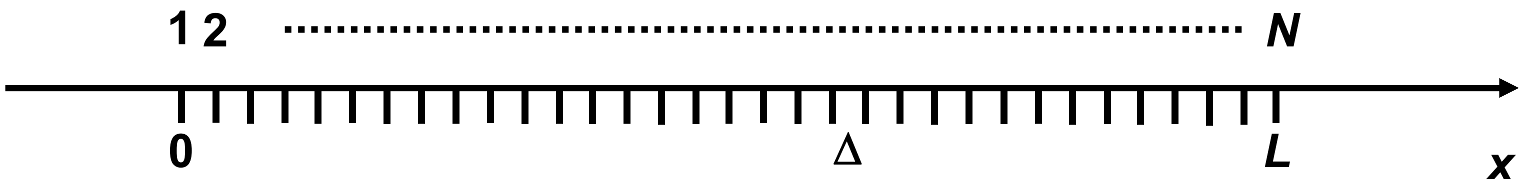
Complete Orthornormal Basis Set: Position Basis



Consider the position basis:

$$
|x_1\rangle = \frac{1}{\Delta}\begin{bmatrix} 1 \\ 0 \\ 0 \\ . \\ . \\ \\ 0 \end{bmatrix} \qquad
|x_2\rangle = \frac{1}{\Delta}\begin{bmatrix} 0 \\ 1 \\ 0 \\ . \\ . \\ \\ 0 \end{bmatrix} \qquad
|x_3\rangle = \frac{1}{\Delta}\begin{bmatrix} 0 \\ 0 \\ 1 \\ . \\ . \\ \\ 0 \end{bmatrix} \qquad \cdots\cdots \qquad
|x_N\rangle = \frac{1}{\Delta}\begin{bmatrix} 0 \\ 0 \\ 0 \\ . \\ . \\ \\ 1 \end{bmatrix}
$$

Complete Orthornormal Basis Set: Position Basis



$$\langle x_j | x_j \rangle = \frac{1}{\Delta^2} [0\ 0\ 0 \ldots\ldots 1 \ldots\ldots 0\ 0\ 0] \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix} \Delta = 1/\Delta$$

$$\langle x_k | x_j \rangle = \frac{1}{\Delta^2} [0\ 0\ 1 \ldots\ldots 0 \ldots\ldots 0\ 0\ 0] \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \\ 0 \\ 0 \end{bmatrix} \Delta = \frac{\delta_{kj}}{\Delta}$$

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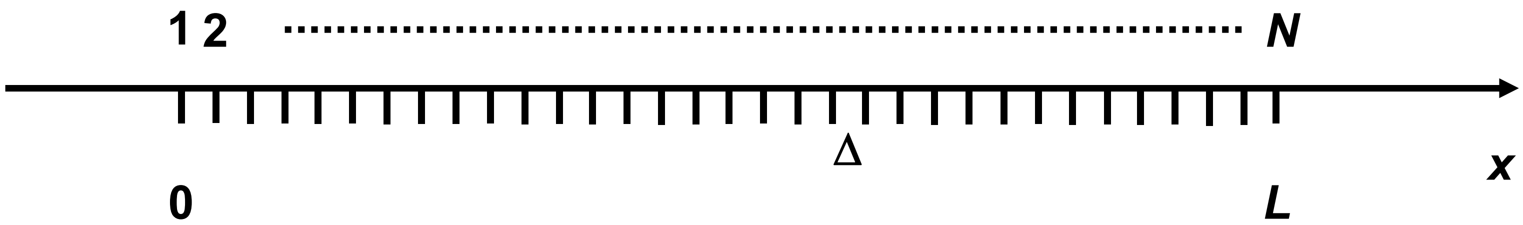

$$|x_1\rangle = \begin{bmatrix} 1/\Delta \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \\ 0 \end{bmatrix} \quad |x_2\rangle = \begin{bmatrix} 0 \\ 1/\Delta \\ 0 \\ \cdot \\ \cdot \\ \\ 0 \end{bmatrix} \quad |x_3\rangle = \begin{bmatrix} 0 \\ 0 \\ 1/\Delta \\ \cdot \\ \cdot \\ \\ 0 \end{bmatrix} \quad \cdots\cdots \quad |x_N\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \\ 1/\Delta \end{bmatrix}$$

Orthogonality:

$$\langle x_k | x_j \rangle = \frac{\delta_{kj}}{\Delta}$$

Completeness:

$$\sum_{j=1}^{N} \Delta |x_j\rangle\langle x_j| = \hat{1}$$

Check!

How to represent an vector $|f\rangle$ in this position basis?

$$|f\rangle = \begin{bmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \\ \\ f_N \end{bmatrix}$$

$$\begin{aligned} |f\rangle &= \hat{1}|f\rangle \\ &= \left(\sum_{j=1}^{N} \Delta |x_j\rangle\langle x_j| \right) |f\rangle \\ &= \sum_{j=1}^{N} \Delta |x_j\rangle\langle x_j|f\rangle \\ &= \sum_{j=1}^{N} \Delta \; f_j |x_j\rangle \end{aligned}$$

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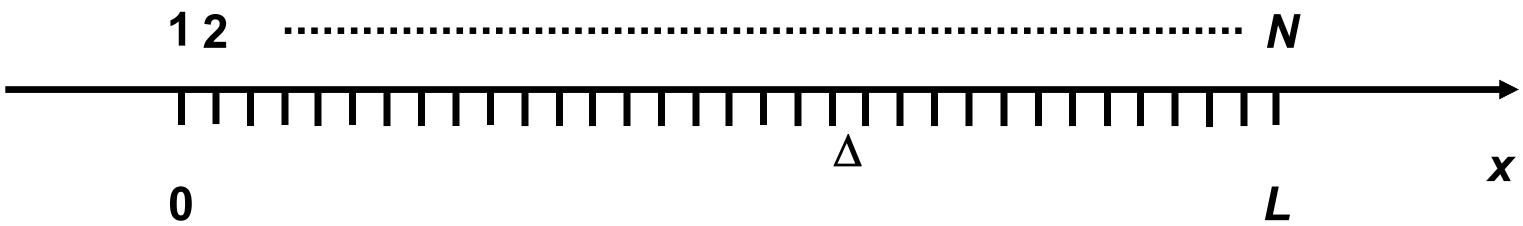


Now take the limit of Δ goes to 0 and *N* goes to ∞ to get:

Orthogonality: $\langle x_k | x_j \rangle = \dfrac{\delta_{kj}}{\Delta} \xrightarrow{Lt\ \Delta \to 0} \langle x' | x \rangle = \delta(x - x')$

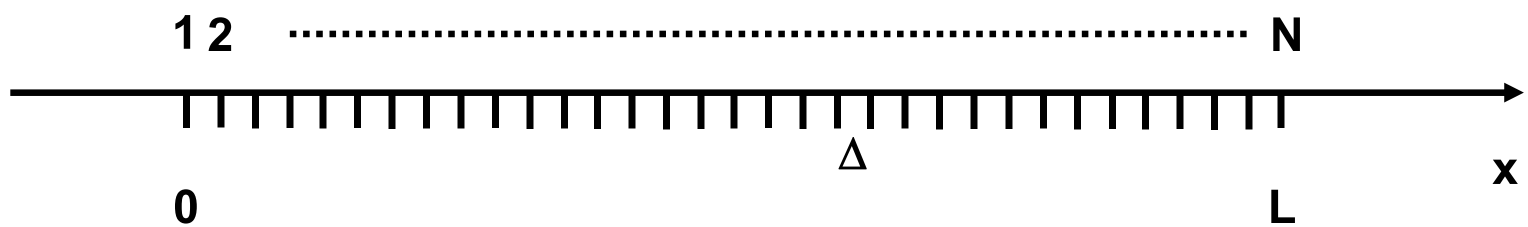
Completeness: $\sum_{j=1}^{N} \Delta | x_j \rangle \langle x_j | = \hat{1} \xrightarrow{Lt\ \Delta \to 0} \int dx\, | x \rangle \langle x | = \hat{1}$

Inner product: $\langle x_j | f \rangle = f_j \xrightarrow{Lt\ \Delta \to 0} \langle x | f \rangle = f(x)$

$\langle f | x_j \rangle = f_j^{*} \xrightarrow{Lt\ \Delta \to 0} \langle f | x \rangle = f^{*}(x)$

Representation: $| f \rangle = \hat{1} | f \rangle = \left(\int dx\, | x \rangle \langle x | \right) | f \rangle = \int dx\, | x \rangle \langle x | f \rangle = \int dx\, f(x) | x \rangle$

Differential Operator



Recall that an operator takes one vector into another vector in the same Hilbert space:

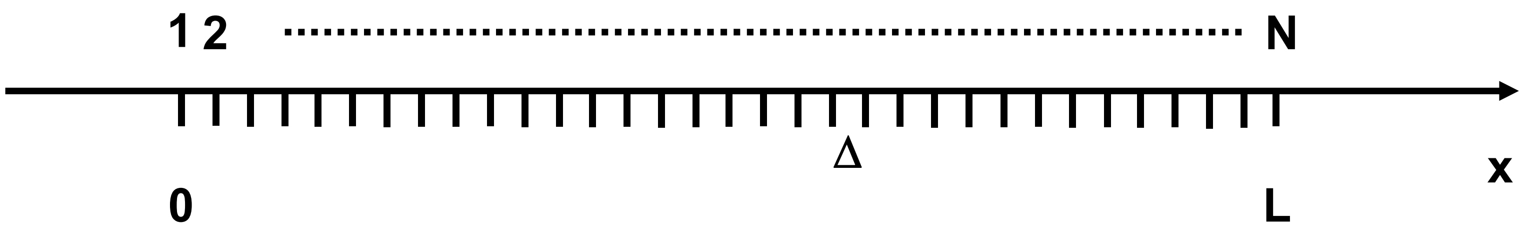
$$\hat{O}|f\rangle = \begin{bmatrix} 0 & 1/2\Delta & & & & & & \\ -1/2\Delta & 0 & 1/2\Delta & & & & & \\ & -1/2\Delta & 0 & 1/2\Delta & & & & \\ & & -1/2\Delta & \vdots & \vdots & & & \\ & & & \vdots & \vdots & 1/2\Delta & & \\ & & & & -1/2\Delta & 0 & 1/2\Delta & \\ & & & & & -1/2\Delta & 0 & 1/2\Delta \\ & & & & & & -1/2\Delta & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ . \\ . \\ . \\ . \\ f_N \end{bmatrix} = \begin{bmatrix} . \\ . \\ \frac{f_j - f_{j-2}}{2\Delta} \\ \frac{f_{j+1} - f_{j-1}}{2\Delta} \\ \frac{f_{j+2} - f_j}{2\Delta} \\ . \\ . \\ . \end{bmatrix}$$

$$\Rightarrow \langle x_j|\hat{O}|f\rangle = \frac{f_{j+1} - f_{j-1}}{2\Delta} \xrightarrow{Lt\ \Delta\to 0} \langle x|\hat{O}|f\rangle = \frac{\partial f(x)}{\partial x}$$

Action of the operator $\hat{O}$ viewed in the position basis

Differential operator!!

Hermitian Differential Operator



Recall that an operator takes one vector into another vector in the same Hilbert space

$$\hat{O}\left|f\right\rangle = \begin{bmatrix} 0 & \hbar/2i\Delta & & & & & & \\ -1/2i\Delta & 0 & \hbar/2i\Delta & & & & & \\ & -\hbar/2i\Delta & 0 & \hbar/2i\Delta & & & & \\ & & -\hbar/2i\Delta & \vdots & \vdots & & & \\ & & & \vdots & \vdots & \hbar/2i\Delta & & \\ & & & & -\hbar/2i\Delta & 0 & \hbar/2i\Delta & \\ & & & & & -\hbar/2i\Delta & 0 & \hbar/2i\Delta \\ & & & & & & -\hbar/2i\Delta & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ . \\ . \\ . \\ . \\ f_N \end{bmatrix} = \begin{bmatrix} . \\ . \\ . \\ \frac{\hbar}{i}\frac{f_{j+1}-f_{j-1}}{2\Delta} \\ . \\ . \\ . \\ . \end{bmatrix}$$

$$\Rightarrow \left\langle x_j \middle| \hat{O} \middle| f \right\rangle = \frac{\hbar}{i}\frac{f_{j+1}-f_{j-1}}{2\Delta} \xrightarrow{Lt\ \Delta\to 0} \left\langle x \middle| \hat{O} \middle| f \right\rangle = \frac{\hbar}{i}\frac{\partial f(x)}{\partial x}$$

Hermitian differential operator!!

Hermitian Differential Operator

Definition of a Hermitian operator

$$\langle g|\hat{O}|f\rangle = \left(\langle f|\hat{O}^\dagger|g\rangle\right)^*$$

Show that this differential operator is Hermitian: $\langle x|\hat{O}|f\rangle = \frac{\hbar}{i}\frac{\partial f(x)}{\partial x}$

Proof:

$$\langle g|\hat{O}|f\rangle = \langle g|\left(\int_0^L dx\,|x\rangle\langle x|\right)\hat{O}|f\rangle = \int_0^L dx\; g^*(x)\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\right]f(x)$$

→ **Integrate by parts**

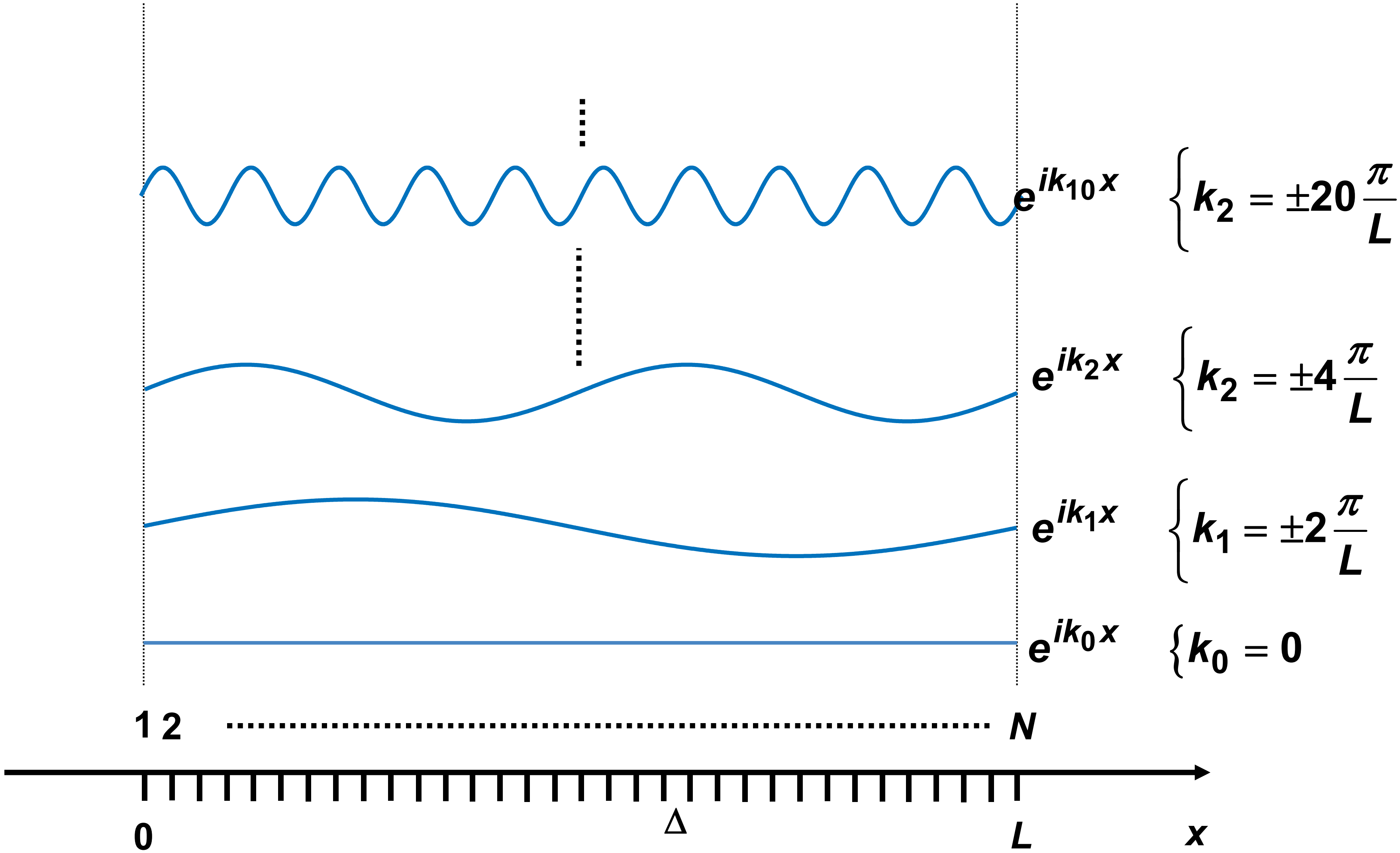
$$= g^*(x)\frac{\hbar}{i}f(x)\Big|_0^L - \int_0^L dx\,\frac{\hbar}{i}\frac{\partial g^*(x)}{\partial x}f(x)$$

$$= \int_0^L dx\,\frac{-\hbar}{i}\frac{\partial g^*(x)}{\partial x}f(x)$$

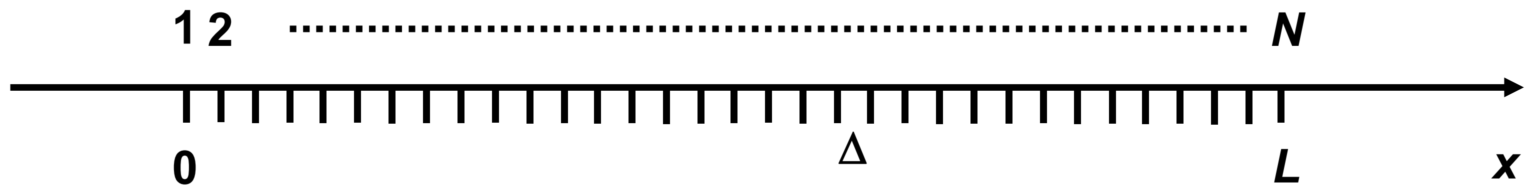
$$= \left[\int_0^L dx\, f^*(x)\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\right]g(x)\right]^* = \left(\langle f|\hat{O}^\dagger|g\rangle\right)^*$$

$$\Rightarrow \quad \hat{O} = \hat{O}^\dagger$$

Another Complete Orthornormal Basis Set: Plane Wave Basis



Another Complete Orthornormal Basis Set: Plane Wave Basis



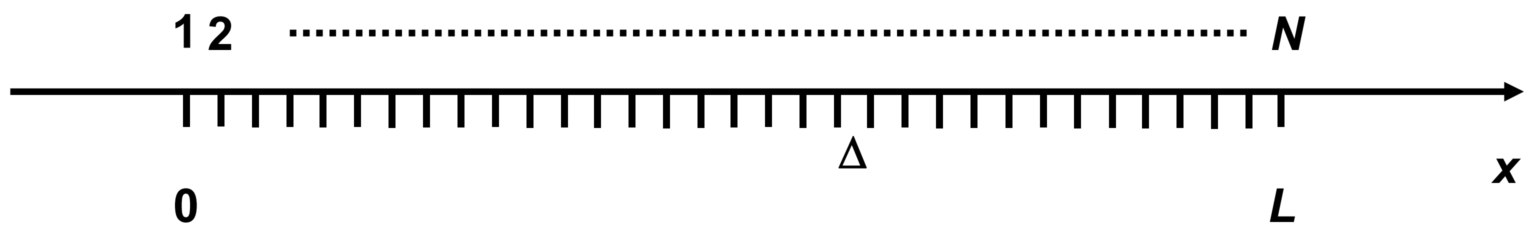
$$|k_1\rangle = \begin{bmatrix} e^{ik_1x_1} \\ e^{ik_1x_2} \\ e^{ik_1x_3} \\ \cdot \\ \cdot \\ \\ e^{ik_1x_N} \end{bmatrix} \quad |k_2\rangle = \begin{bmatrix} e^{ik_2x_1} \\ e^{ik_2x_2} \\ e^{ik_2x_3} \\ \cdot \\ \cdot \\ \\ e^{ik_2x_N} \end{bmatrix} \quad |k_3\rangle = \begin{bmatrix} e^{ik_3x_1} \\ e^{ik_3x_2} \\ e^{ik_3x_3} \\ \cdot \\ \cdot \\ \\ e^{ik_3x_N} \end{bmatrix} \quad \cdots\cdots \quad |k_N\rangle = \begin{bmatrix} e^{ik_Nx_1} \\ e^{ik_Nx_2} \\ e^{ik_Nx_3} \\ \cdot \\ \cdot \\ \\ e^{ik_Nx_N} \end{bmatrix}$$

$$k_n = \frac{2\pi}{L} n \qquad \langle k_n | k_m \rangle = L\delta_{nm} \qquad \langle x_m | k_n \rangle = e^{ik_nx_m} \qquad \sum_j \frac{1}{L} |k_j\rangle\langle k_j| = \hat{1}$$

$\{ \; n = -N/2, \ldots -1, 0, 1, \ldots\ldots N/2 - 1$

***N* different *k* values are possible => *N* different basis vectors**

Another Complete Orthornormal Basis Set: Plane Wave Basis



$$|k\rangle = \begin{bmatrix} e^{ikx_1} \\ e^{ikx_2} \\ e^{ikx_3} \\ \cdot \\ \cdot \\ \\ e^{ikx_N} \end{bmatrix}$$

Orthogonality: $\langle k_n | k_m \rangle = L\delta_{nm} \xrightarrow{Lt\ \Delta\to 0} \langle k' | k \rangle = 2\pi\delta(k-k')$

Completeness: $\sum_j \frac{1}{L} |k_j\rangle\langle k_j| = \hat{1} \xrightarrow{Lt\ \Delta\to 0} \int_{-\infty}^{\infty} \frac{dk}{2\pi} |k\rangle\langle k| = \hat{1}$

Inner product: $\langle x_j | k_n \rangle = e^{ik_n x_j} \xrightarrow{Lt\ \Delta\to 0} \langle x | k \rangle = e^{ikx}$

Representation:

$$|f\rangle = \hat{1}|f\rangle = \left(\int_{-\infty}^{\infty} \frac{dk}{2\pi} |k\rangle\langle k| \right)|f\rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} |k\rangle\langle k|f\rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} f(k)|k\rangle$$

$$\Rightarrow \langle x|f\rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi} f(k)\langle x|k\rangle$$

$$\Rightarrow f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} f(k)e^{ikx}$$

→ Fourier Transform!!

Plane Wave Basis Completeness Relation: Proof

$$\sum_j \frac{1}{L}\left|k_j\right\rangle\left\langle k_j\right| = \hat{1} \xrightarrow{Lt\ \Delta\to 0} \int_{-\infty}^{\infty} \frac{dk}{2\pi}\left|k\right\rangle\left\langle k\right| = \hat{1}$$

$$\left|k_1\right\rangle = \begin{bmatrix} e^{ik_1x_1} \\ e^{ik_1x_2} \\ e^{ik_1x_3} \\ \cdot \\ \cdot \\ \\ e^{ik_1x_N} \end{bmatrix} \quad \left|k_2\right\rangle = \begin{bmatrix} e^{ik_2x_1} \\ e^{ik_2x_2} \\ e^{ik_2x_3} \\ \cdot \\ \cdot \\ \\ e^{ik_2x_N} \end{bmatrix} \quad \left|k_3\right\rangle = \begin{bmatrix} e^{ik_3x_1} \\ e^{ik_3x_2} \\ e^{ik_3x_3} \\ \cdot \\ \cdot \\ \\ e^{ik_3x_N} \end{bmatrix} \quad \cdots\cdots\cdots\cdots \quad \left|k_N\right\rangle = \begin{bmatrix} e^{ik_Nx_1} \\ e^{ik_Nx_2} \\ e^{ik_Nx_3} \\ \cdot \\ \cdot \\ \\ e^{ik_Nx_N} \end{bmatrix}$$

$$k_n = \frac{2\pi}{L} n$$

$$\{\ n = -N/2, \ldots -1, 0, 1, \ldots\ldots N/2 - 1$$

$$\Delta k = k_{n+1} - k_n = \frac{2\pi}{L}$$

$$\sum_j \frac{1}{L}\left|k_j\right\rangle\left\langle k_j\right| = \hat{1}$$

$$\Rightarrow \sum_j \frac{\Delta k}{\Delta k}\frac{1}{L}\left|k_j\right\rangle\left\langle k_j\right| = \hat{1}$$

$$\Rightarrow \sum_j \frac{\Delta k}{\left(\frac{2\pi}{L}\right)}\frac{1}{L}\left|k_j\right\rangle\left\langle k_j\right| = \hat{1}$$

$$\Rightarrow \sum_j \frac{\Delta k}{2\pi}\left|k_j\right\rangle\left\langle k_j\right| = \hat{1}$$

$$\Rightarrow \int_{-\infty}^{\infty} \frac{dk}{2\pi}\left|k\right\rangle\left\langle k\right| = \hat{1}$$

Operator Representations

The action of operators look very different in different basis!

Consider this operator (discussed earlier):

$$\langle x|\hat{O}|f\rangle = \frac{\hbar}{i}\frac{\partial f(x)}{\partial x}$$

We need to find how the action of the operator appears in the plane wave basis:

$$\langle k|\hat{O}|f\rangle = ?$$

$$= \langle k|\hat{1}\,\hat{O}|f\rangle$$

$$= \langle k|\int_{-\infty}^{\infty} dx\,|x\rangle\langle x|\hat{O}|f\rangle$$

$$= \int_{-\infty}^{\infty} dx\,\langle k|x\rangle\langle x|\hat{O}|f\rangle = \int_{-\infty}^{\infty} dx\; e^{-ikx}\,\frac{\hbar}{i}\frac{\partial f(x)}{\partial x}$$

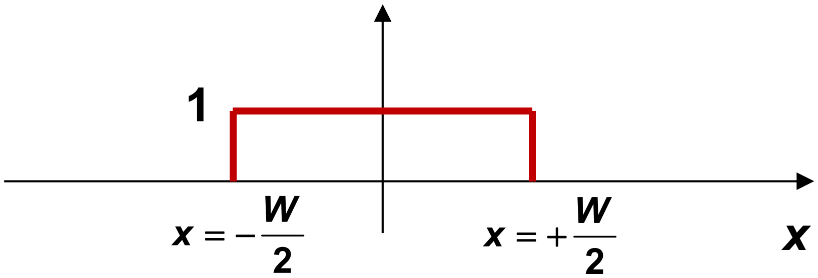
→ Integrate by parts

$$= \hbar k \int_{-\infty}^{\infty} dx\; e^{-ikx} f(x)$$

$$= \hbar k\;\; f(k) = \hbar k\,\langle k|f\rangle$$

How to Think About Things When Doing Quantum Physics

Consider a function *f*(*x*):



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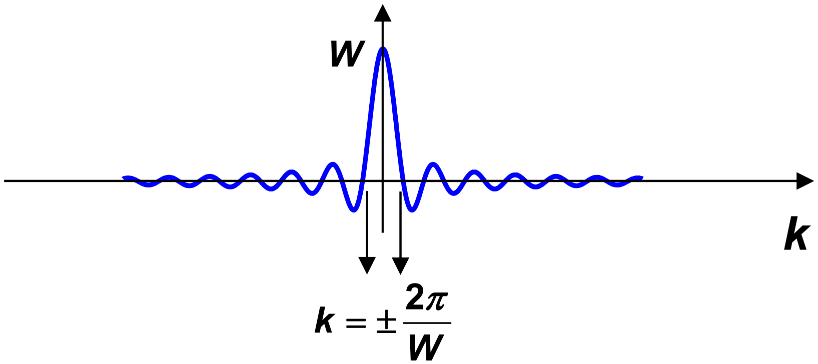
Consider Fourier Transform of *f*(*x*):



$$f(k) = \int_{-\infty}^{\infty} dx\, e^{-ikx} f(x) = W\,\frac{\sin(kW/2)}{kW/2}$$

The way you should think about this is to consider *f* a vector in a Hilbert space:

$$|f\rangle$$

The vector $|f\rangle$ is the real deal. Everything else is a representation of $|f\rangle$ in different basis:

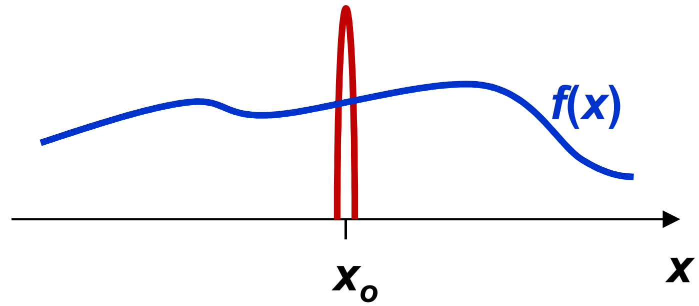
$$f(k) = \langle k|f\rangle$$

$$f(x) = \langle x|f\rangle$$

Delta Functions in 1D and 3D

A delta function in 1D has the following property:

$$\int_{-\infty}^{\infty} dx\, f(x)\,\delta(x - x_o) = f(x_o)$$



Integration of plane waves over all space (in 1D):

$$\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = 2\pi\,\delta(k - k')$$

A delta function in 3D has the following property:

$$\int d^3\vec{r}\, f(\vec{r})\,\delta^3(\vec{r} - \vec{r}_o) = f(\vec{r}_o)$$

$$\delta^3(\vec{r} - \vec{r}_o) = \delta(x - x_o)\,\delta(y - y_o)\,\delta(z - z_o)$$

Integration of a plane waves over all space (in 3D):

$$\int d^3\vec{r}\, e^{i(\vec{k}-\vec{k}').\vec{r}} = (2\pi)^3\,\delta^3(\vec{k} - \vec{k}')$$