6. Functions of Operators

HAT: A FUNCTION OF A LIN. OP. IS ITSELF A LIN. OP.

Let $\hat{\Omega}$ be a lin. op. on $\mathbb{V}^n(\mathbb{C})$

We can define a Function of $\hat{\Omega}$ formally, via a Taylor Series Expansion: $\hat{f}(\hat{\Omega}) \equiv \sum_{p=0}^{\infty} a_p \hat{\Omega}^p, \quad a_p \in \mathbb{C}$

IMPT. EXAMPLE:

$$e^{\hat{\Omega}} \equiv \sum_{p=0}^{\infty} \frac{\hat{\Omega}^p}{p!} = \underset{\substack{\Uparrow \\ \text{Formal def.} \\ \text{of } \hat{\Omega}^0}}{\hat{\mathbb{I}}} + \frac{1}{1!}\hat{\Omega} + \frac{1}{2!}\hat{\Omega}\cdot\hat{\Omega} + \dots$$

Product of operators: Becomes ordinary Matrix Multiplication in an orthonormal basis

$$\langle i|\hat{\Omega}\hat{\Omega}|j\rangle = \langle i|\hat{\Omega}\,\hat{\mathbb{I}}\,\hat{\Omega}|j\rangle = \sum_{k=1}^{n} \langle i|\hat{\Omega}|k\rangle\langle k|\hat{\Omega}|j\rangle$$

$$= \Omega_{ik}\Omega_{kj} \quad \left(\begin{smallmatrix}\text{Einstein} \\ \text{sum on} \\ k=1,3,\dots,n\end{smallmatrix}\right)$$

Further: Assume $\hat{\Omega}^\dagger = \hat{\Omega}$ Hermitian

$\therefore$ In the $\{|\omega_i\rangle\}$ eigenbasis $\hat{\Omega}|\omega_i\rangle = \omega_i|\omega_i\rangle$

$$\hat{\Omega} \Rightarrow \begin{bmatrix} \omega_1 & & & 0 \\ & \omega_2 & & \\ & & \ddots & \\ 0 & & & \omega_n \end{bmatrix} ; \quad \hat{\Omega}^p \Rightarrow \begin{bmatrix} \omega_1^p & & & 0 \\ & \omega_2^p & & \\ & & \ddots & \\ 0 & & & \omega_n^p \end{bmatrix}$$

Lec. 4, p5; This Lec. 5, p1

$$\therefore e^{\hat{\Omega}} = \sum_{p=0}^{\infty} \frac{1}{p!}\hat{\Omega}^p \Rightarrow \begin{bmatrix} e^{\omega_1} & & & \\ & e^{\omega_2} & & \\ & & \ddots & \\ 0 & & & e^{\omega_n} \end{bmatrix}$$

$\Rightarrow$ Generalizes to any Analytic Function $f(z)$: $\hat{f}(\hat{\Omega}) = \text{diag}\{f(\omega_1), f(\omega_2), \dots, f(\omega_n)\}$

For $\hat{\Omega} = \hat{\Omega}^\dagger$

Functions of non-commuting operators do not commute, nor follow ordinary rules for composition of $\mathbb{C}$-number functions!

Consider

$$e^{\lambda\hat{A}} e^{\lambda\hat{B}} = \left(\hat{\mathbb{I}} + \lambda\hat{A} + \frac{\lambda^2}{2!}\hat{A}^2 + \dots\right)\left(\hat{\mathbb{I}} + \lambda\hat{B} + \frac{\lambda^2}{2!}\hat{B}^2 + \dots\right)$$

$$= \hat{\mathbb{I}} + \lambda(\hat{A}+\hat{B}) + \frac{\lambda^2}{2!}\left(\hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2\right) + \mathcal{O}(\lambda^3)$$

$$= \hat{\mathbb{I}} + \lambda(\hat{B}+\hat{A}) + \frac{\lambda^2}{2!}\left(\hat{B}^2 + 2\hat{B}\hat{A} + \hat{A}^2 + 2[\hat{A},\hat{B}]\right) + \mathcal{O}(\lambda^3)$$

$$\neq e^{\lambda\hat{B}} e^{\lambda\hat{A}}$$

UNLESS

$$[\hat{A},\hat{B}] = 0$$

Functions of Operators... Continued

$$e^{\lambda\hat{A}}e^{\lambda\hat{B}} \neq e^{\lambda\hat{B}}e^{\lambda\hat{A}} \quad \text{if } [\hat{A},\hat{B}] \neq 0$$

Composition Rule for a Product of Exp. Functions of Lin. Ops $\hat{A},\hat{B}$:

"Baker-Campbell-Hausdorff" Formula

$$e^{\lambda\hat{A}}\cdot e^{\lambda\hat{B}} = e^{\lambda(\hat{A}+\hat{B}) + \frac{\lambda^2}{2}[\hat{A},\hat{B}] + \frac{\lambda^3}{12}\left([\hat{A},[\hat{A},\hat{B}]]+[\hat{B},[\hat{B},\hat{A}]]\right) + O(\lambda^4)} \Leftarrow \text{Infinite series of nested commutators}$$

① We will not prove this here. You will prove a related formula in HW

② Two special cases:

a) $[\hat{A},\hat{B}]=0 \implies e^{\lambda\hat{A}}e^{\lambda\hat{B}} = e^{\lambda(\hat{A}+\hat{B})}$, as if $\hat{A},\hat{B}$ are ordinary numbers (instead of operators)

b) $[\hat{A},\hat{B}] = i\alpha\hat{\mathbb{I}}$, $\alpha\in\mathbb{C}$

$$\implies e^{\lambda\hat{A}}e^{\lambda\hat{B}} = e^{\lambda(\hat{A}+\hat{B})}e^{\frac{\lambda^2}{2}[\hat{A},\hat{B}]} = e^{\lambda(\hat{A}+\hat{B})}e^{\frac{\lambda^2}{2}i\alpha}$$

$$= e^{\lambda\hat{B}}e^{\lambda\hat{A}}e^{\lambda^2[\hat{A},\hat{B}]}$$ Useful in Quantum!

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③ Technical Note/Observation: (Not essential for this class)

Let $\hat{U}_A \equiv e^{\hat{A}}$, etc. Then $\hat{U}_A\cdot\hat{U}_B = \hat{U}_C$

$\hat{C} = \hat{A}+\hat{B} + \{$ infinite sum of nested commutators of $\hat{A},\hat{B}$

$\implies$ If a set of operators $\{\hat{A}_i\}$ closes under commutation,

i.e. $[\hat{A}_i,\hat{A}_j] = \sum_{k=1}^{N} f_{ijk}\hat{A}_k \Leftarrow$ This is called a "Lie Algebra"

f_{ijk}: "structure constants"

Then: $$e^{\alpha_i\hat{A}_i}e^{\beta_j\hat{A}_j} = e^{\gamma_k\hat{A}_k}$$ (sum on all repeated indices)

"Lie Group": Product of any two exponentials of "generators" $\{\hat{A}_i\}$ is itself an exponential of $\{\hat{A}_j\}$

We will not study Lie Groups in general, but we will study SO(3), SU(2) Lie Groups in context of SPIN

LEMMA: EXPONENTIAL OF AN ANTIHERMITIAN OPERATOR IS UNITARY

IMPORTANT!

LET $\hat{\Omega} \equiv -i\hat{H}$, $\hat{H}^{+} = \hat{H} \Rightarrow \hat{\Omega}^{+} = -\hat{\Omega}$ ANTIHERMITIAN

WORK IN ORTHONORMAL EIGENBASIS OF $\hat{H}$: $\hat{H}|\varepsilon_i\rangle = \varepsilon_i |\varepsilon_i\rangle$, $\varepsilon_i^* = \varepsilon_i$

$\langle \varepsilon_i | \varepsilon_j \rangle = \delta_{ij}$

THEN $\hat{U} \equiv e^{-i\hat{H}} \Rightarrow \begin{bmatrix} e^{-i\varepsilon_1} & & & 0 \\ & e^{-i\varepsilon_2} & & \\ & & \ddots & \\ 0 & & & e^{-i\varepsilon_n} \end{bmatrix}$

$\therefore \hat{U}^{+}\hat{U} = \hat{\mathbb{I}}$ ✓

DERIVATIVE OF A LINEAR OPERATOR

SUPPOSE $\hat{\Omega} = \hat{\Omega}(\lambda)$ IS A LIN. OP. THAT DEPENDS ON THE $\mathbb{C}$-VALUED (OR REAL) PARAMETER λ

DERIVATIVE OF $\hat{\Omega}(\lambda)$ WITH RESPECT TO λ: $\quad \dfrac{d\hat{\Omega}(\lambda)}{d\lambda} \equiv \lim_{\Delta\lambda \to 0} \dfrac{\hat{\Omega}(\lambda+\Delta\lambda) - \hat{\Omega}(\lambda)}{\Delta\lambda}$

IN SOME ORTHONORMAL BASIS:

$$\frac{d\hat{\Omega}}{d\lambda} \Rightarrow \begin{bmatrix} \frac{d\Omega_{11}}{d\lambda} & \frac{d\Omega_{12}}{d\lambda} & \cdots & \frac{d\Omega_{1n}}{d\lambda} \\ \frac{d\Omega_{21}}{d\lambda} & & & \\ \vdots & & & \vdots \\ \frac{d\Omega_{n1}}{d\lambda} & \cdots & & \frac{d\Omega_{nn}}{d\lambda} \end{bmatrix}$$

$\Rightarrow \therefore$ IN GENERAL,

$$\left[\hat{\Omega}(\lambda), \frac{d}{d\lambda}\hat{\Omega}(\lambda)\right] \neq 0 \,!$$

OPERATOR AND ITS DERIV. W.R.T. A PARAMETER λ DO NOT COMMUTE

IMPORTANT EXAMPLE

LET $\hat{U} \equiv e^{-i\hat{H}t}$; $\quad i\dfrac{d}{dt}\hat{U} = i\dfrac{d}{dt}e^{-i\hat{H}t}$

$$= i\frac{d}{dt}\left(\sum_{p=0}^{\infty} \frac{(-it)^p}{p!}\hat{H}^p\right)$$

$$= \hat{H}\hat{U} = \hat{U}\hat{H} \quad \left(\text{SINCE } [\hat{H},\hat{U}]=0\right)$$

$\therefore \left(i\dfrac{d}{dt} - \hat{H}\right)\hat{U} = 0$ HAS SOLUTION $\hat{U} = e^{-it\hat{H}}$; $\hat{U}^{+}\hat{U} = \hat{\mathbb{I}}$ IF $\hat{H}^{+} = \hat{H}$

⊛ Must be careful with Op. order in general

ex: $\frac{d}{d\lambda}\left(e^{\lambda\hat{\Omega}} e^{\lambda\hat{\Theta}}\right) = \hat{\Omega}\, e^{\lambda\hat{\Omega}} e^{\lambda\hat{\Theta}} + e^{\lambda\hat{\Omega}} e^{\lambda\hat{\Theta}}\, \hat{\Theta}$ "ordered" chain rule

Must preserve order of non-commuting factors [⇒ matrices in an orthonormal basis]

Almost done with Math Intro! One more (important) topic:

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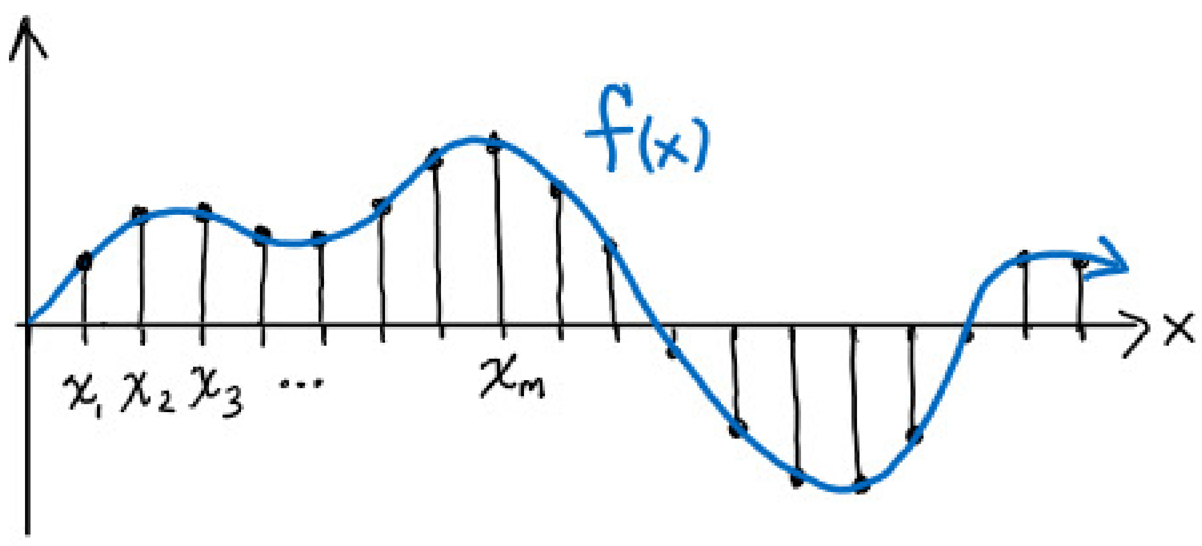
⑦ Infinite-Dimensional Vector Spaces ("Hilbert Spaces")



Consider a "well-behaved" function $f(x)$ over some interval on the real line

"Well-behaved": ① square-normalizable "L^2"

$$\int dx\, |f(x)|^2 = \text{finite}$$

or

② "delta-function normalizable" (later...)

Approximation to $f(x)$:

Sample at regular intervals $\{x_m\}$, $x_n \equiv n a$ ← integer (n); sampling interval (a) ("lattice spacing")

E.g., take $1 \le n \le N$, such that $a \le x_m \le Na \equiv L$

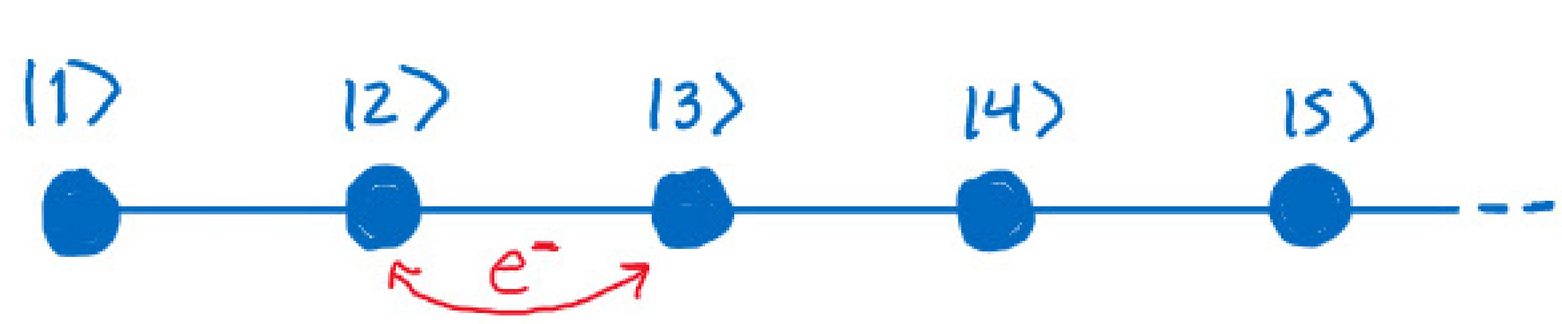
Orthonormal basis: "lattice sites" $\{|x_m\rangle\}$ $\quad \langle x_m | x_n \rangle = \delta_{mn}$

$$|x_p\rangle \Rightarrow \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow p^{\text{th}} \text{ place}$$

Let $f_N(x_m) \equiv f(x_m)$, N-times "sampled" function

$$|f_N\rangle \Rightarrow \begin{bmatrix} f_N(x_1) \\ f_N(x_2) \\ \vdots \\ f_N(x_N) \end{bmatrix} ; \quad \langle x_m | f_N \rangle = f_N(x_m)$$

- This discrete approximation is actually useful in certain contexts:
  - Digital (e.g. audio) signals with a fixed sampling rate (44KHz)
  - "Tight-binding" models in solid-state physics: approximate electrons moving in a crystalline solid as "hopping" from atom to atom



$|2\rangle\langle 3| + |3\rangle\langle 2|$ ⇐ operator that "hops" between atoms 2, 3

- $|f_N\rangle = \sum_{i=1}^{N} f_N(x_i)|x_i\rangle = \sum_{i=1}^{N} |x_i\rangle\langle x_i|f_N\rangle$; IDENTITY OPERATOR $\hat{\mathbb{I}} = \sum_{i=1}^{N} |x_i\rangle\langle x_i|$

- INNER PRODUCT:

$$\langle f_N|g_N\rangle = \langle f_N|\hat{\mathbb{I}}|g_N\rangle = \sum_{i=1}^{N} \langle f_N|x_i\rangle\langle x_i|g_N\rangle = \sum_{i=1}^{N} f_N^*(x_i)\, g_N(x_i)$$

← ALLOWING FOR $\mathbb{C}$-VALUED FUNCTIONS OF x

- $a \le x_i \le Na \equiv L$ ⟶ IN DISCRETE CASE, ALL WORKS AS EXPECTED IN $\mathbb{V}^N(\mathbb{C})$

"CONTINUUM LIMIT": WANT TO TAKE "LATTICE SPACING" $a \to 0$, $N \to \infty$, SUCH THAT

$0 \le x \le L$, $L = Na$ REMAINS FINITE

$\Rightarrow$ DISCRETE POINTS $\{x_i\}$ "SQUEEZE TOGETHER," MERGE INTO CONTINUUM OF x OVER $[0,L]$
(WILL DISCUSS INFINITE INTERVALS LATER)

$$|x_i\rangle \in \mathbb{V}^N(\mathbb{C}) \xrightarrow[N\to\infty]{a\to 0} |x\rangle \in \mathbb{V}^\infty(\mathbb{C})$$

⟸ AN "INFINITE-DIMENSIONAL" VECTOR SPACE

$\mathbb{V}^\infty(\mathbb{C})$ IS A COMPLICATED OBJECT. LET'S TRY TO UNDERSTAND IT BY NAIVE GENERALIZATION FROM $\mathbb{V}^N$.

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1. $\langle x_i|f_N\rangle = f_N(x_i) = f(x_i) \Longrightarrow \langle x|f\rangle = f(x)$

2. $\hat{\mathbb{I}} = \sum_{i=1}^{N} |x_i\rangle\langle x_i| \Longrightarrow \hat{\mathbb{I}} = \int_0^L |x'\rangle\langle x'|\, dx'$

   x': INTEGRATION VARIABLE

3. INNER PRODUCTS:

$$\langle f_N|g_N\rangle = \sum_{i=1}^{N} \langle f_N|x_i\rangle\langle x_i|g_N\rangle = \sum_{i=1}^{N} f_N^*(x_i)\, g_N(x_i)$$

$$\Downarrow$$

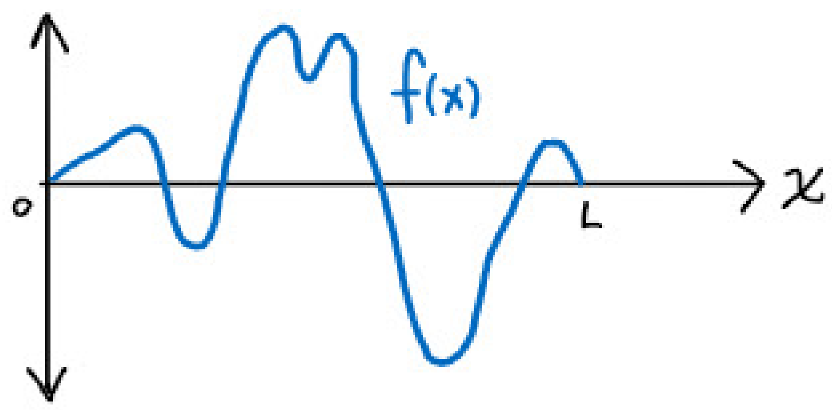
$$\langle f|g\rangle = \langle f|\hat{\mathbb{I}}|g\rangle = \int_0^L dx\, \langle f|x\rangle\langle x|g\rangle = \int_0^L dx\, f^*(x)\, g(x)$$

4. NORMALIZATION OF BASIS VECTORS

$$\langle x_i|f_N\rangle = f_N(x_i) = \langle x_i|\hat{\mathbb{I}}|f_N\rangle = \sum_{j=1}^{N} \langle x_i|x_j\rangle\langle x_j|f_N\rangle$$

$$\langle x_i|x_j\rangle = \delta_{ij} = \begin{cases} 1, & i=j \\ 0, & i\neq j \end{cases}$$ "KRONECKER" (DISCRETE) DELTA FUNCTION

Continuous $|x\rangle$ Basis



$$\langle x|f\rangle = f(x) = \langle x|\hat{\mathbb{I}}|f\rangle = \int_0^L dx' \, \langle x|x'\rangle\langle x'|f\rangle$$

$$= \int_0^L dx' \, \langle x|x'\rangle \, f(x')$$

Dirac (Continuum) Delta Function

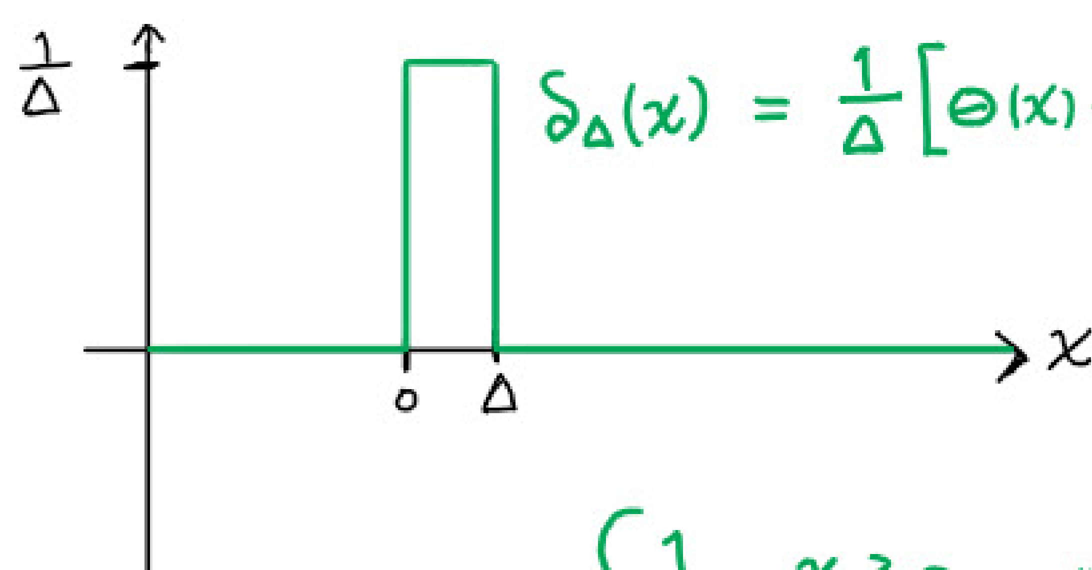
Let $\langle x|x'\rangle \equiv \delta(x-x')$ "Dirac Delta Function"

Defining Properties:

① $$\int_{-\infty}^{\infty} dx \, \delta(x-x_0) f(x) = f(x_0)$$ • Picks up value of $f(x)$ only at $x = x_0$

② $$\int_{-\infty}^{\infty} dx \, \delta(x-x_0) = 1$$ • Normalization

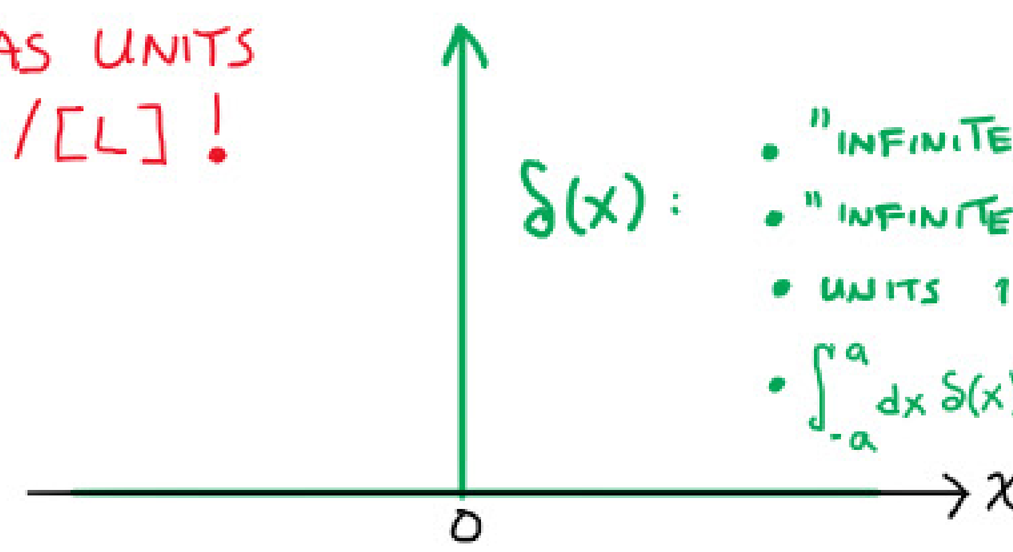
Can be Viewed as a Limit:



$$\delta_\Delta(x) = \frac{1}{\Delta}\left[\Theta(x) - \Theta(x-\Delta)\right]$$

Has units $1/[L]$!

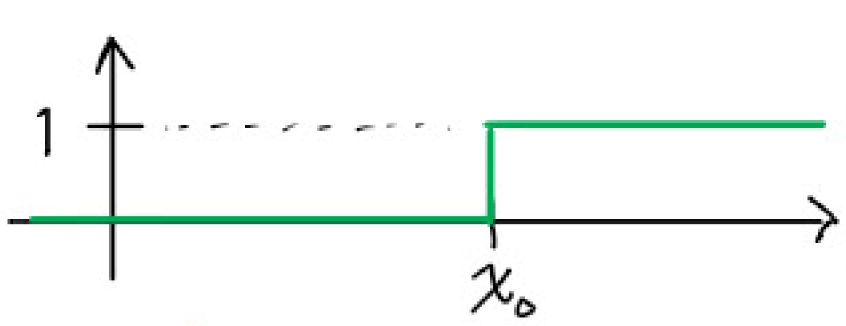
$$\xRightarrow[\Delta\to 0]{\lim}$$



$\delta(x)$:

- "Infinitely Narrow"
- "Infinitely Tall"
- Units $1/[L]$
- $\int_{-a}^{a} dx \, \delta(x) = 1$ for any $a > 0$

$$\Theta(x) \equiv \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$ "Heaviside" Unit Step Function



- Piecewise Continuous
- Can be viewed as a limit:

$$\Theta(x) = \lim_{\Delta\to 0} \frac{1}{2}\left[1 + \tanh\left(\frac{x}{\Delta}\right)\right]$$

Dirac Delta Function: Derivative of $\Theta(x)$

From the definition,

$$\delta_\Delta(x) = \frac{1}{\Delta}\left[\Theta(x) - \Theta(x-\Delta)\right]$$

$$\Downarrow \quad \Delta \to 0$$

$$\delta(x) = \frac{d}{dx}\Theta(x)$$

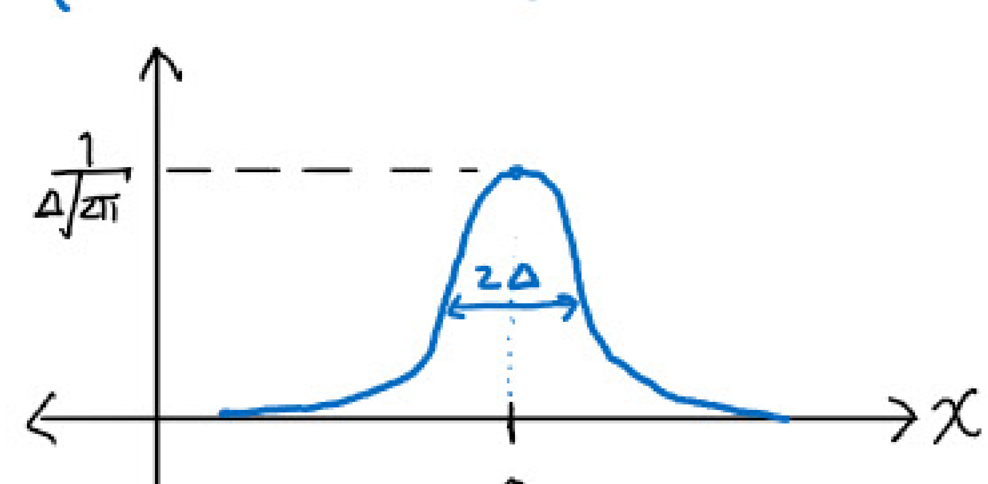
- $\delta = 0$ for $x \neq 0$
- $\delta \to \infty$ at $x = 0$ due to ∞ slope of $\Theta(x)$ there

Since $\delta(x)$ is defined by its properties ①, ② under integ., no unique way to define via limiting process.

Other "Models":

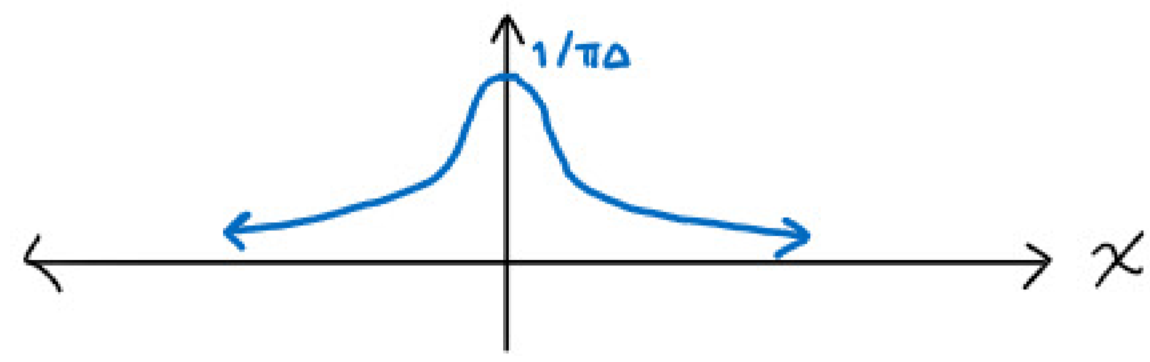
① Gaussian

$$\delta_\Delta(x) = \frac{1}{\Delta\sqrt{2\pi}} e^{-\frac{x^2}{2\Delta^2}}$$



② LORENTZIAN ("CAUCHY DISTRIBUTION")

$$\delta_\Delta(x) = \frac{\left(\frac{\Delta}{\pi}\right)}{x^2 + \Delta^2}$$



$\Rightarrow$ RECTANGULAR PULSE, GAUSSIAN, LORENTZIAN MODELS ALL GIVE DIFFERENT RESULTS FOR

$$I_\Delta(x_0) \equiv \int_{-\infty}^{\infty} dx \;\; \delta_\Delta(x - x_0)\; f(x)$$

BUT IN $\Delta \to 0$ LIMIT, ASSUMING $f(x)$ IS "WELL-BEHAVED" (e.g., SQUARE-INTEGRABLE), $I_\Delta(x_0) \xrightarrow{\lim \Delta \to 0} f(x_0)$, <u>REGARDLESS</u> OF THE MODEL FOR $\delta_\Delta(x)$

TECHNICALLY, $\delta(x)$ IS A "GENERALIZED FUNCTION" OR "DISTRIBUTION"