Quantum Mechanics

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Lesson I
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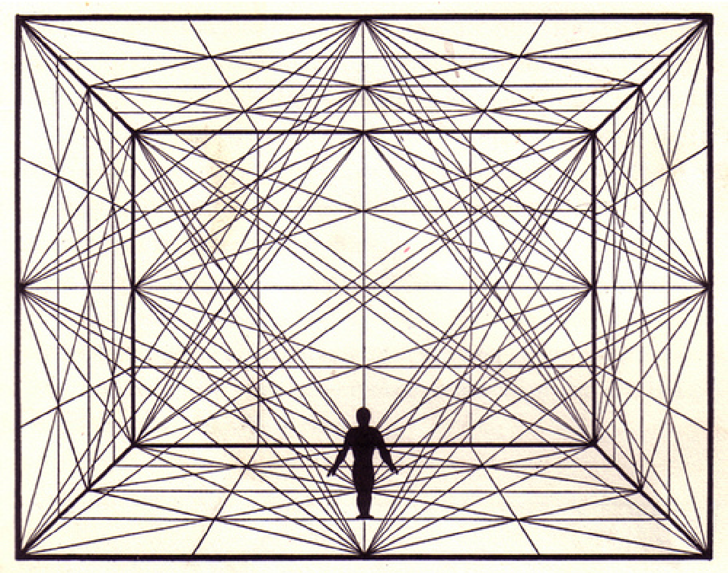
Linear Spaces



Definition 1: A *field* is a set F together with two operations $+$ and $\cdot$ for which all the axioms below hold $\forall\ \lambda,\ \mu,\ \nu \in F$:

- closure $\to$ the sum $\lambda + \mu$ and the product $\lambda \cdot \mu$ again belong to F
- associative law $\to$ $\lambda + (\mu + \nu) = (\lambda + \mu) + \nu$ and $\lambda \cdot (\mu \cdot \nu) = (\lambda \cdot \mu) \cdot \nu$
- commutative law $\to$ $\lambda + \nu = \nu + \lambda$ and $\lambda \cdot \mu = \mu \cdot \lambda$
- distributive laws $\to$ $\lambda \cdot (\mu + \nu) = \lambda \cdot \mu + \lambda \cdot \nu$ and $(\lambda + \mu) \cdot \nu = \lambda \cdot \nu + \mu \cdot \nu$
- existence of an additive identity $\to$ there exists an element $0 \in F$ for which $\lambda + 0 = \lambda$
- existence of a multiplicative identity $\to$ there exists an element $1 \in F$, with $1 \neq 0$ for which $1 \cdot \lambda = \lambda$
- existence of additive inverse $\to$ to every $\lambda \in F$, there corresponds an additive inverse $-\lambda$, such that $-\lambda + \lambda = 0$
- existence of multiplicative inverse $\to$ to every $\lambda \in F$, there corresponds a multiplicative inverse λ^{-1}, such that $\lambda^{-1} \cdot \lambda = 1$

Example: $\mathbb{R}$ and $\mathbb{C}$

Definition 2: A *vector space* over the field F is a set V on which two operations are defined (called addition $+$ and scalar multiplication $\cdot$) that must satisfy the axioms below $\forall\, x, y, w \in V$ and $\forall\, \lambda, \mu \in F$:

- closure $\rightarrow$ the sum $x + y$ and the scalar multiplication $\lambda \cdot x$ are uniquely defined and belong to V
- commutative law of vector addition $\rightarrow$ $x + y = y + x$
- associative law of vector addition $\rightarrow$ $x + (y + w) = (x + y) + w$
- existence of an additive identity $\rightarrow$ there exists an element $\mathbf{0} \in V$ such that $x + \mathbf{0} = x$
- existence of additive inverses $\rightarrow$ to every element $x \in V$ there corresponds an inverse element $-x$, such that $-x + x = \mathbf{0}$
- associative law of scalar multiplication $\rightarrow$ $(\lambda \cdot \mu) \cdot x = \lambda \cdot (\mu \cdot x)$
- distributive laws of scalar multiplication $\rightarrow$ $(\lambda + \mu) \cdot x = \lambda \cdot x + \mu \cdot x$ and $\lambda \cdot (x + y) = \lambda \cdot x + \lambda \cdot y$
- unitary law $\rightarrow$ $1 \cdot x = x$

Example: For any field F ☞ set F^n of n-tuples is vector space over F

Cartesian space $\mathbb{R}^n$ ☞ prototypical example of real n-dimensional V:

Let $\boldsymbol{x} = (x_1, \cdots, x_n)$ be an ordered n-tuple of real numbers x_i, to which there corresponds a point $\boldsymbol{x}$ with these Cartesian coordinates and a vector $\boldsymbol{x}$ with these components. We define addition of vectors by component addition

$$\boldsymbol{x} + \boldsymbol{y} = (x_1 + y_1, \cdots, x_n + y_n)$$

and scalar multiplication by component multiplication

$$\lambda\, \boldsymbol{x} = (\lambda x_1, \cdots, \lambda x_n)$$

Definition 3: Given a vector space V over a field F, a subset W of V is called a subspace if W is a vector space over F under the operations already defined on V

- After defining notions of vector spaces and subspaces ☞ next step is to identify functions that can be used to relate one vector space to another
- These functions should respect algebraic structure of vector spaces ☞ so it is reasonable to require that they preserve addition and scalar multiplication

Definition 4: Let V and W be vector spaces over the field F. A linear transformation from V to W is a function $T : V \to W$ such that

$$T(\lambda \boldsymbol{x} + \mu \boldsymbol{y}) = \lambda T(\boldsymbol{x}) + \mu T(\boldsymbol{y})$$

for all vectors $\boldsymbol{x}, \boldsymbol{y} \in V$ and all scalars $\lambda, \mu \in F$. If a linear transformation is one-to-one and onto, it is called a vector space isomorphism, or simply an isomorphism.

Definition 5: Let $S = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\}$ be a set of vectors in the vector space V over the field F. Any vector of the form $\boldsymbol{y} = \sum_{i=1}^{n} \lambda_i \boldsymbol{x}_i$, for $\lambda_i \in F$, is called a linear combination of the vectors in S. The set S is said to span V if each element of V can be expressed as a linear combination of the vectors in S.

Definition 6: Let $\boldsymbol{x_1}, \cdots, \boldsymbol{x_m}$ be m given vectors and $\lambda_1, \cdots \lambda_m$ an equal number of scalars. Then we can form a linear combination or sum

$$\lambda_1 \boldsymbol{x_1} + \cdots + \lambda_k \boldsymbol{x_k} + \cdots + \lambda_m \boldsymbol{x_m}$$

which is also an element of the vector space. Suppose there exist values $\lambda_1 \cdots \lambda_n$, which are not all zero, such that the above vector sum is the zero vector. Then the vectors $\boldsymbol{x_1}, \cdots, \boldsymbol{x_m}$ are said to be *linearly dependent*. Contrarily, the vectors $\boldsymbol{x_1}, \cdots, \boldsymbol{x_m}$ are called *linearly independent* if

$$\lambda_1 \boldsymbol{x_1} + \cdots + \lambda_k \boldsymbol{x_k} + \cdots + \lambda_m \boldsymbol{x_m} = \boldsymbol{0}$$

demands the scalars λ_k must all be zero.

Definition 7: The dimension of V is the maximal number of linearly independent vectors of V

Definition 8: Let V be an n dimensional vector space and

$$S = \{\boldsymbol{x_1}, \cdots, \boldsymbol{x_n}\} \subset V$$

a linearly independent spanning set for V ☞ S is called a basis of V

Definition 9: An inner product $\langle\, , \rangle : V \times V \to F$ is a function that takes each ordered pair (x, y) of elements of V to a number $\langle x, y\rangle \in F$ and has the following properties:

- conjugate symmetry or Hermiticity $\to$ $\langle \boldsymbol{x}, \boldsymbol{y}\rangle = (\langle \boldsymbol{y}, \boldsymbol{x}\rangle)^*$
- linearity in the second argument $\to$ $\langle \boldsymbol{x}, \boldsymbol{y}+\boldsymbol{w}\rangle = \langle \boldsymbol{x}, \boldsymbol{y}\rangle + \langle \boldsymbol{x}, \boldsymbol{w}\rangle$ and $\langle \boldsymbol{x}, \lambda\, \boldsymbol{y}\rangle = \lambda \langle \boldsymbol{x}, \boldsymbol{y}\rangle$
- definiteness $\to$ $\langle \boldsymbol{x}, \boldsymbol{x}\rangle = 0 \Leftrightarrow \boldsymbol{x} = 0$

Definition 10: An inner product $\langle\, , \rangle$ is said to be positive definite $\Leftrightarrow$ for all non-zero $\boldsymbol{x}$ in V, $\langle \boldsymbol{x}, \boldsymbol{x}\rangle \geq 0$

Definition 11: An inner product space is a vector space V over the field F equipped with an inner product $\langle\, , \rangle : V \times V \to F$

Definition 12: The vector space V on F endowed with a positive definite inner product (a.k.a. scalar product) defines the Euclidean space $\mathscr{E}$

Example: For $x, y \in \mathbb{R}^n$ ☞ $\langle \boldsymbol{x}, \boldsymbol{y}\rangle = \boldsymbol{x}\cdot\boldsymbol{y} = \sum_{k=1}^n x_k y_k$

Example: For $x, y \in \mathbb{C}^n$ ☞ $\langle \boldsymbol{x}, \boldsymbol{y}\rangle = \boldsymbol{x}\cdot\boldsymbol{y} = \sum_{k=1}^n x_k^* y_k$

Example:

- Let $\mathcal{C}([a,b])$ denote the set of continuous functions $x(t)$ defined on the closed interval $-\infty < a \leq t \leq b < \infty$
- This set is structured as a vector space with respect to the usual operations of sum of functions and product of functions by numbers, whose neutral element is the zero function
- For $x(t), y(t) \in \mathcal{C}([a,b])$ ☞ we can define the scalar product: $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \int_a^b x^*(t)\, y(t)\, dt$ which satisfies all the necessary axioms
- In particular ☞ $\langle \boldsymbol{x}, \boldsymbol{x} \rangle = \int_a^b |x(t)|^2 dt \geq 0$ and if $\langle \boldsymbol{x}, \boldsymbol{x} \rangle = 0$ then $0 = \int_a^b |x(t)|^2\, dt \geq \int_{a_1}^{b_1} |x(t)|^2\, dt \geq 0\ \forall a \leq a_1 \leq b_1 \leq b$ therefore ☞ $x(t) \equiv 0$
- Indeed ☞ since $x(t)$ is continuous, if $x(t_0) \neq 0$ with $a \leq t_0 \leq b$ then $x(t) \neq 0$ in an interval of such point ☞ contradiction

Definition 13: The axiom of positivity allows one to define a norm or length for each vector of an euclidean space

$$\|\boldsymbol{x}\| = +\sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$$

- In particular ☞ $\|\boldsymbol{x}\| = 0 \Leftrightarrow \boldsymbol{x} = \mathbf{0}$
- Further ☞ if $\lambda \in \mathbb{C}$ then $\|\lambda \boldsymbol{x}\| = \sqrt{|\lambda|^2 \langle \boldsymbol{x}, \boldsymbol{x} \rangle} = |\lambda| \|\boldsymbol{x}\|$
- This allows a normalization for any non-zero length vector
- Indeed ☞ if $\boldsymbol{x} \neq \mathbf{0}$ then $\|\boldsymbol{x}\| > 0$
- Thus ☞ we can take $\lambda \in \mathbb{C}$ such that $|\lambda| = \|x\|^{-1}$ and $\boldsymbol{y} = \lambda \boldsymbol{x}$
- It follows that $\|\boldsymbol{y}\| = |\lambda| \|\boldsymbol{x}\| = 1$.

Example: The length of a vector $\boldsymbol{x} \in \mathbb{R}^n$ is

$$\|\boldsymbol{x}\| = \left(\sum_{k=1}^{n} x_k^2 \right)^{1/2}$$

Example: The length of a vector $\boldsymbol{x} \in \mathcal{C}^2([a, b])$ is

$$\|\boldsymbol{x}\| = \left\{ \int_a^b |x(t)|^2 \, dt \right\}^{1/2}$$

Definition 14: In a real Euclidean space the angle between the vectors x and y is defined by

$$\cos \widehat{xy} = \frac{|\langle x, y \rangle|}{\|x\| \|y\|}$$

Definition 15: Two vectors are orthogonal, $x \perp y$, if $\langle x, y \rangle = 0$. The zero vector is orthogonal to every vector in $\mathscr{E}$.

Definition 16: In a real Euclidean space the angle between two orthogonal non-zero vectors is $\pi/2$, *i.e.* $\cos \widehat{xy} = 0$

Definition 17: The angle between two complex vectors is given by

$$\cos \widehat{xy} = \frac{\mathrm{Re}(|\langle x, y \rangle|)}{\|x\| \|y\|}$$

Definition 18: A basis $x_1, \cdots, x_n$ of $\mathscr{E}$ is called orthogonal if $\langle x_i, x_j \rangle = 0$ for all $i \neq j$. The basis is called *orthonormal* if, in addition, each vector has unit length, *i.e.*, $\|x_i\| = 1$, $\forall i = 1, \cdots, n$.

Example: Simplest example of orthonormal basis is standard basis

$$\boldsymbol{e_1} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{e_2} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \quad \cdots \quad \boldsymbol{e_n} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

Definition 19: A Hilbert space $\mathscr{H}$ is a vector space that

- has an inner product
- is "complete" ☞ which means limits work nicely

Hilbert spaces are possibly-infinite-dimensional analogues of the finite-dimensional Euclidean spaces

Example: Any finite dimensional inner product space is $\mathscr{H}$

Example: The space l^2 of infinite sequences of complex numbers

$l^2 = \{(x_1, x_2, x_3, \cdots) : x_k \in \mathbb{C}, \sum_{k=1}^{\infty} |x_k|^2 < \infty\}$ with $\langle y, x \rangle = \sum_{k=1}^{\infty} y_k^* x_k$

Example: The space $\mathcal{L}^2$ defined by the collection of measurable real or complex valued square integrable functions

$$\int_{-\infty}^{\infty} |\psi(t)|^2 \, dt < \infty$$

endowed with inner product

$$\langle \Psi, \Phi \rangle = \int_a^b \psi^*(t) \, \phi(t) \, dt$$

and associated norm

$$\|\Psi\| = \left\{ \int_{-\infty}^{\infty} |\psi(t)|^2 \, dt \right\}^{1/2}$$

is an infinite dimensional Hilbert space $\mathscr{H}$

Linear Operators on Euclidean Spaces

Definition 20:

- An operator A on $\mathscr{E}$ is a vector function $A : \mathscr{E} \to \mathscr{E}$
- The operator is called linear if

$$A(\alpha \boldsymbol{x} + \beta \boldsymbol{y}) = \alpha A \boldsymbol{x} + \beta A \boldsymbol{y}, \ \forall \boldsymbol{x}, \boldsymbol{y} \in \mathscr{E} \text{ and } \forall \alpha, \beta \in \mathbb{C} \text{ (or } \mathbb{R})$$

Definition 21: Let $\mathbb{A}$ be an $n \times n$ matrix and $\boldsymbol{x}$ a vector:

- the function $A(\boldsymbol{x}) = \mathbb{A}\boldsymbol{x}$ is obviously a linear operator
- a vector $\boldsymbol{x} \neq \mathbf{0}$ is an eigenvector of $\mathbb{A}$ if $\exists\, \lambda$ satisfying $\mathbb{A}\,\boldsymbol{x} = \lambda\, \boldsymbol{x}$
- in such a case ☞ $(\mathbb{A} - \lambda\, \mathbb{1})\, \boldsymbol{x} = \mathbf{0}$ with $\mathbb{1}$ the identity matrix
- eigenvalues λ are given by the relation $\det\, (\mathbb{A} - \lambda\, \mathbb{1}) = 0$ which has m different roots with $1 \leq m \leq n$ (note that $\det(\mathbb{A} - \lambda\, \mathbb{1})$ is a polynomial of degree n)
- The eigenvectors associated with the eigenvalue λ can be obtained by solving the (singular) linear system $(\mathbb{A} - \lambda\, \mathbb{1})\, \boldsymbol{x} = \mathbf{0}$

Definition 22: A complex square matrix $\mathbb{A}$ is Hermitian if $\mathbb{A} = \mathbb{A}^\dagger$
☞ $\mathbb{A}^\dagger = (\mathbb{A}^*)^T$ is the conjugate transpose of a complex matrix

Definition 23: A linear operator A on a Hilbert space $\mathscr{H}$ is symmetric if $\langle A\boldsymbol{x}, \boldsymbol{y}\rangle = \langle \boldsymbol{x}, A\boldsymbol{y}\rangle$, $\forall\, \boldsymbol{x}$ and $\boldsymbol{y}$ in the domain of A

Definition 24: A symmetric everywhere defined operator is called self-adjoint or Hermitian

Example: If we take as $\mathscr{H}$ the Hilbert space $\mathbb{C}^n$ with the standard dot product and interpret a Hermitian square matrix $\mathbb{A}$ as a linear operator on $\mathscr{H}$ ☞ we have: $\langle \boldsymbol{x}, \mathbb{A}\boldsymbol{y}\rangle = \langle \mathbb{A}\boldsymbol{x}, \boldsymbol{y}\rangle, \forall\, \boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^n$

Definition 25: Dirac delta function as a limit

- Consider the function

$$g_\epsilon(x) = \begin{cases} 1/\epsilon & |x| \leq \epsilon/2 \\ 0 & |x| > \epsilon/2 \end{cases}$$

  with $\epsilon > 0$
- It follows that $\int_{-\infty}^{+\infty} g_\epsilon(x)\, dx = 1 \ \forall \epsilon > 0$
- In addition ☞ if f is an arbitrary continuous function

$$\int_{-\infty}^{+\infty} g_\epsilon(x)\, f(x) dx = \epsilon^{-1} \int_{-\epsilon/2}^{+\epsilon/2} f(x)\, dx = \frac{F(\epsilon/2) - F(-\epsilon/2)}{\epsilon},$$

  where F is the primitive of f
- For $\epsilon \to 0^+$ ☞ $g_\epsilon(x)$ is concentrated near the origin yielding

$$\lim_{\epsilon \to 0^+} \int_{-\infty}^{+\infty} g_\epsilon(x) f(x)\, dx = \lim_{\epsilon \to 0^+} \frac{F(\epsilon/2) - F(-\epsilon/2)}{\epsilon} = F'(0) = f(0)$$

- We can define the distribution (or generalized function) as the limit

$$\delta(x) = \lim_{\epsilon \to 0^+} g_\epsilon(x)$$

satisfying

$$\int_{-\infty}^{+\infty} \delta(x)\, f(x)\, dx = f(0)$$

- Although limit $\delta(x)$ does not strictly exist

  (it is 0 if $x \neq 0$ and ∞ if $x = 0$)

  limit of integral $\exists\ \forall f$ continuous in an interval centered at $x = 0$

  and this is the meaning of $\delta(x)$
- We will consider from now on test functions f
  which are bounded and differentiable functions to any order
  and which vanish outside a finite range I
- Remember first and foremost that such functions exist ☞ e.g.

  if $f(x) = 0$, for $x \leq 0$ and $x \geq 1$

  and $f(x) = e^{-1/x^2} e^{-1/(1-x)^2}$, for $|x| < 1$

  then the function f has derivatives of any order at $x = 0$ and $x = 1$

- Many other $g_\epsilon(x)$ converge to $\delta(x)$ ☞ with derivatives of all orders
- A well-known example ☞ $\delta(x) = \lim_{\epsilon\to 0^+} \frac{e^{-x^2/2\epsilon^2}}{\sqrt{2\pi}\epsilon}$
- Indeed ☞

$$\frac{1}{\sqrt{2\pi}\epsilon}\int_{-\infty}^{+\infty} e^{-x^2/2\epsilon^2} dx = 1 \;\forall \epsilon > 0$$

  and

$$\lim_{\epsilon\to 0^+} \frac{1}{\sqrt{2\pi}\epsilon}\int_{-\infty}^{+\infty} e^{-x^2/2\epsilon^2} f(x) dx = f(0)$$

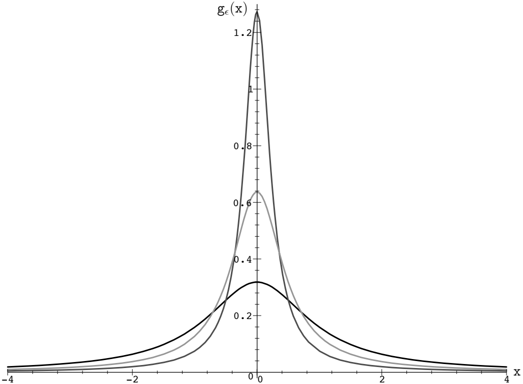
- Here ☞

$$g_\epsilon(x) = \frac{1}{\sqrt{2\pi}\,\epsilon} e^{-x^2/2\epsilon^2}$$

  is the normal (or Gaussian) distribution of area 1 and variance

$$\int_{-\infty}^{+\infty} g_\epsilon\, x^2\, dx = \epsilon^2$$

- When $\epsilon \to 0^+$ ☞ $g_\epsilon(x)$ concentrates around $x = 0$ keeping its area constant



The delta function as a limit in the sense of distributions

Definition 26: The convolution of $\delta(x)$ with other functions is defined in such a way that the integration rules still hold

- For example ☞

$$\int_{-\infty}^{+\infty} \delta(x-x_0)f(x)dx = \int_{-\infty}^{+\infty} \delta(u)\ f(u+x_0)du = f(x_0)$$

- Similarly ☞ if $a \neq 0$

$$\int_{-\infty}^{+\infty} \delta(ax)f(x)dx = \frac{1}{|a|}\int_{-\infty}^{+\infty} \delta(u)\ f(u/a)du = \frac{1}{|a|}f(0)$$

  and so

$$\delta(ax) = \frac{1}{|a|}\delta(x) \quad a \neq 0\,.$$

- In particular ☞ $\delta(-x) = \delta(x)$

Definition 27: Integration by parts

- If we want δ to fulfill the usual equalities of integration by parts we must define the derivative

$$\int_{-\infty}^{+\infty} \delta'(x)\, f(x)\, dx = -\int_{-\infty}^{+\infty} \delta(x)\, f'(x)\, dx = -f'(0)\,,$$

  recalling that $f = 0$ outside a finite interval
- In general ☞

$$\int_{-\infty}^{+\infty} \delta^{(n)}(x)\, f(x)\, dx = (-1)^n f^{(n)}(0)$$

  - $f'(x_0) = -\int_{-\infty}^{+\infty} \delta'(x - x_0)\, f(x) dx$
  - $f^{(n)}(x_0) = (-1)^n \int_{-\infty}^{+\infty} \delta^{(n)}(x - x_0)\, f(x)\, dx$
- If $a \neq 0$ ☞

$$\delta^{(n)}(ax) = \frac{1}{a^n |a|} \delta^{(n)}(x)$$

- In particular ☞ $\delta^{(n)}(-x) = (-1)^n \delta^{(n)}(x)$

Corollary ☞ Heaviside function: The step (Heaviside) function

$$\Theta(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}$$

is the "primitive" (at least in symbolic form) of $\delta(x)$

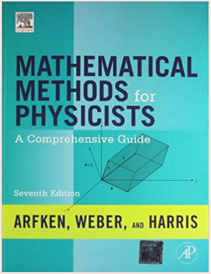
Equivalently ☞ $\Theta'(x)$ has the symbolic limit $\delta(x)$

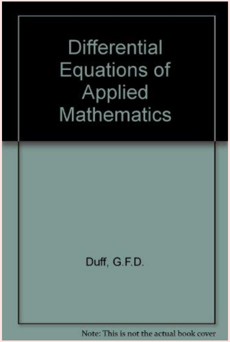
PROOF. For any given test function $f(x)$ ☞ integration by parts leads to

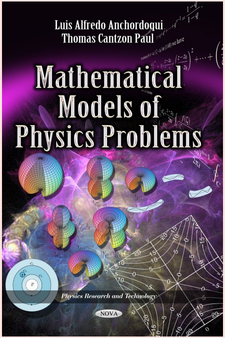
$$\int_{-\infty}^{+\infty} \Theta'(x)\, f(x)\, dx = -\int_{-\infty}^{+\infty} \Theta(x) f'(x)\, dx = -\int_{0}^{\infty} f'(x)\, dx = f(0)$$

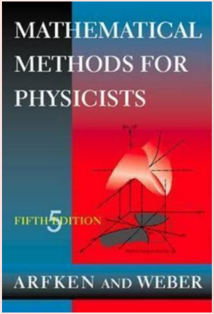
therefore $\Theta'(x) = \delta(x)$

Bibliography









1. G. F. D. Duff and D. Naylor; ISBN: 978-0471223672
2. G. B. Arfken and H. J. Weber; ISBN: 978-0080916729
3. L. A. Anchordoqui and T. C. Paul; ISBN: 978-1626186002