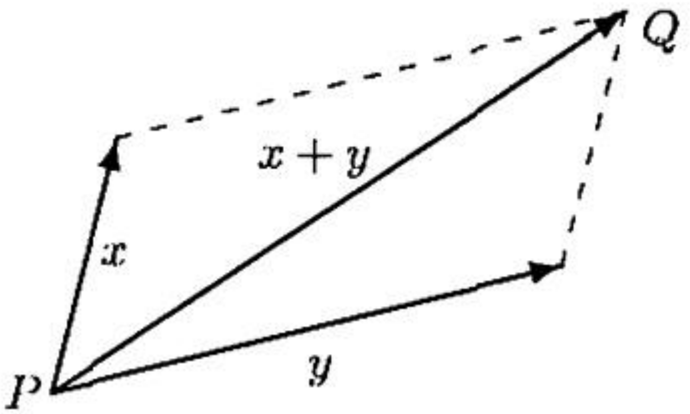
Mathematical Formalism

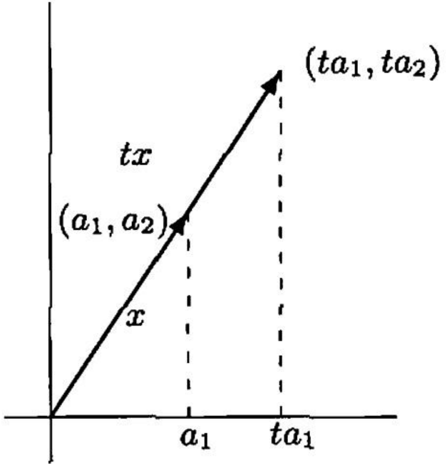
Edrick

Vector Spaces: Motivation

- Vectors (x & y) in $\mathbb{R}^3$ with scalars (a & b) in $\mathbb{R}$



$$x + y = y + x$$
$$(x + y) + z = x + (y + z)$$
$$x + 0 = x$$
$$x + y = 0$$



$$1x = x$$
$$(ab)x = a(bx)$$
$$a(x + y) = ax + ay$$
$$(a + b)x = ax + bx$$

Vector Spaces

Definition 1.2.1 (Vector space) *Consider a nonempty set V, equipped with operations of addition and scalar multiplication. Assume that the following rules are satisfied:*

(i) *For all* $\mathbf{v}, \mathbf{w} \in V$, *we have that* $\mathbf{v} + \mathbf{w} = \mathbf{w} + \mathbf{v}$;

(ii) *For all* $\mathbf{v}, \mathbf{w}, \mathbf{u} \in V$, *we have that* $(\mathbf{v} + \mathbf{w}) + \mathbf{u} = \mathbf{v} + (\mathbf{w} + \mathbf{u})$;

(iii) *There exists an element, called* $\mathbf{0}$, *in* V, *such that for all* $\mathbf{v} \in V$,

$$\mathbf{v} + \mathbf{0} = \mathbf{v};$$

(iv) *For each* $\mathbf{v} \in V$ *there exists an element, called* $-\mathbf{v}$, *in* V, *with the property that*

$$\mathbf{v} + (-\mathbf{v}) = \mathbf{0};$$

(v) *For all* $\alpha, \beta \in \mathbb{C}$ *and all* $\mathbf{v} \in V$,

$$\alpha(\beta\mathbf{v}) = (\alpha\beta)\mathbf{v};$$

(vi) *For all* $\alpha, \beta \in \mathbb{C}$ *and all* $\mathbf{v} \in V$,

$$(\alpha + \beta)\mathbf{v} = \alpha\mathbf{v} + \beta\mathbf{v};$$

(vii) *For all* $\alpha \in \mathbb{C}$ *and all* $\mathbf{v}, \mathbf{w} \in V$,

$$\alpha(\mathbf{v} + \mathbf{w}) = \alpha\mathbf{v} + \alpha\mathbf{w};$$

(viii) *For all* $\mathbf{v} \in V$,

$$1\mathbf{v} = \mathbf{v}.$$

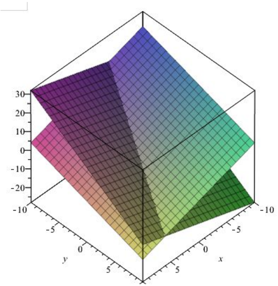
In that case we say that V, equipped with the operations of addition and scalar multiplication, forms a vector space.

Vector Spaces: Examples

- $\mathbb{R}^n$ and $\mathbb{C}^n$
- Matrices $\mathsf{M}_{m\times n}(F)$
- Functions $f : \mathbb{R} \to \mathbb{C}$
- Square-Integrable functions $L^2(\mathbb{R}) = \left\{ f : \mathbb{R} \to \mathbb{C} \mid \int_{-\infty}^{\infty} |f(x)|^2 \, dx < \infty \right\}$
- "Zero vector space" $\mathsf{V} = \{0\}$

Vector Spaces: Additional concepts

- Subspaces



$L^2(\mathbb{R})$ $\qquad$ $A^t = A$

- Linear Independence & dependence

$$\alpha_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \cdots + \alpha_N\mathbf{v}_N = \mathbf{0} \Rightarrow \alpha_1 = \alpha_2 = \cdots = \alpha_N = 0$$

- Bases & dimension

Inner product spaces

Complex conjugation

Definition 4.1.1 (Inner product space) *Let V be a (complex) vector space. An inner product on V is a mapping*

$$\langle \cdot, \cdot \rangle : V \times V \to \mathbb{C} \tag{4.1}$$

for which

(i) $\langle \alpha \mathbf{v} + \beta \mathbf{w}, \mathbf{u} \rangle = \alpha \langle \mathbf{v}, \mathbf{u} \rangle + \beta \langle \mathbf{w}, \mathbf{u} \rangle, \ \forall\, \mathbf{v}, \mathbf{w}, \mathbf{u} \in V, \ \alpha, \beta \in \mathbb{C}$*;*

(ii) $\langle \mathbf{v}, \mathbf{w} \rangle = \overline{\langle \mathbf{w}, \mathbf{v} \rangle}, \ \forall\, \mathbf{v}, \mathbf{w} \in V$*;*

(iii) $\langle \mathbf{v}, \mathbf{v} \rangle \geq 0, \ \forall\, \mathbf{v} \in V$*, and* $\langle \mathbf{v}, \mathbf{v} \rangle = 0 \Leftrightarrow \mathbf{v} = \mathbf{0}$.

A vector space equipped with an inner product is called an inner product space.

Different convention in physics!

$$\begin{aligned} \langle \mathbf{v}, \alpha \mathbf{w} + \beta \mathbf{u} \rangle &= \overline{\langle \alpha \mathbf{w} + \beta \mathbf{u}, \mathbf{v} \rangle} \\ &= \overline{\alpha \langle \mathbf{w}, \mathbf{v} \rangle + \beta \langle \mathbf{u}, \mathbf{v} \rangle} \\ &= \overline{\alpha} \langle \mathbf{v}, \mathbf{w} \rangle + \overline{\beta} \langle \mathbf{v}, \mathbf{u} \rangle, \ \forall\, \mathbf{v}, \mathbf{w}, \mathbf{u} \in V, \ \alpha, \beta \in \mathbb{C}. \end{aligned}$$

Inner product spaces: Examples

- $\mathbb{R}^n$ and $\mathbb{C}^n$

$$\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{k=1}^{n} x_k y_k, \ \mathbf{x}, \mathbf{y} \in \mathbb{R}^n \qquad\qquad \langle \mathbf{x}, \mathbf{y} \rangle = \sum_{k=1}^{n} x_k \overline{y_k}, \ \mathbf{x}, \mathbf{y} \in \mathbb{C}^n$$

- $L^2(\mathbb{R})$

$$\langle f, g \rangle = \int_{-\infty}^{\infty} f(x)\overline{g(x)}\, dx, \ f, g \in L^2(\mathbb{R})$$

- $\mathsf{M}_{n \times n}(F)$

conjugate transpose or Hermitian conjugate

$$\langle A, B \rangle = \operatorname{tr}(B^* A) \qquad A, B \in \mathsf{M}_{n \times n}(F)$$

Inner product spaces: Additional concepts

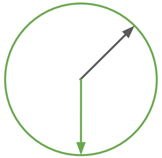
- Orthogonality & Norm

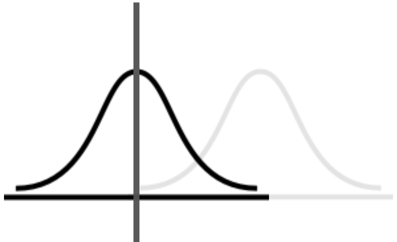
$$\langle \mathbf{v}, \mathbf{w} \rangle = 0 \qquad\qquad ||\mathbf{v}|| := \sqrt{\langle \mathbf{v}, \mathbf{v} \rangle}$$

- Orthonormal Basis

- Orthogonal and Unitary operators

T linear operator and $||Tv|| = ||v||$



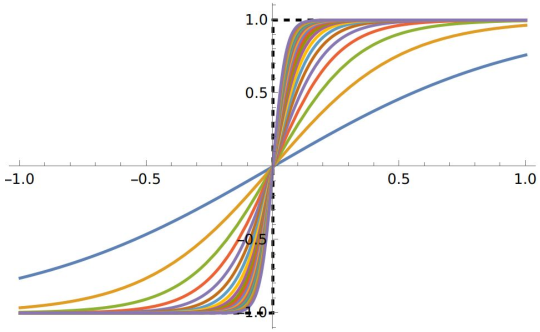


Hilbert Spaces

- A **complete** inner product space is called a **Hilbert space**.

- Completeness

  3 , 3.1, 3.14, 3.141, 3.1415, 3.14159, ...

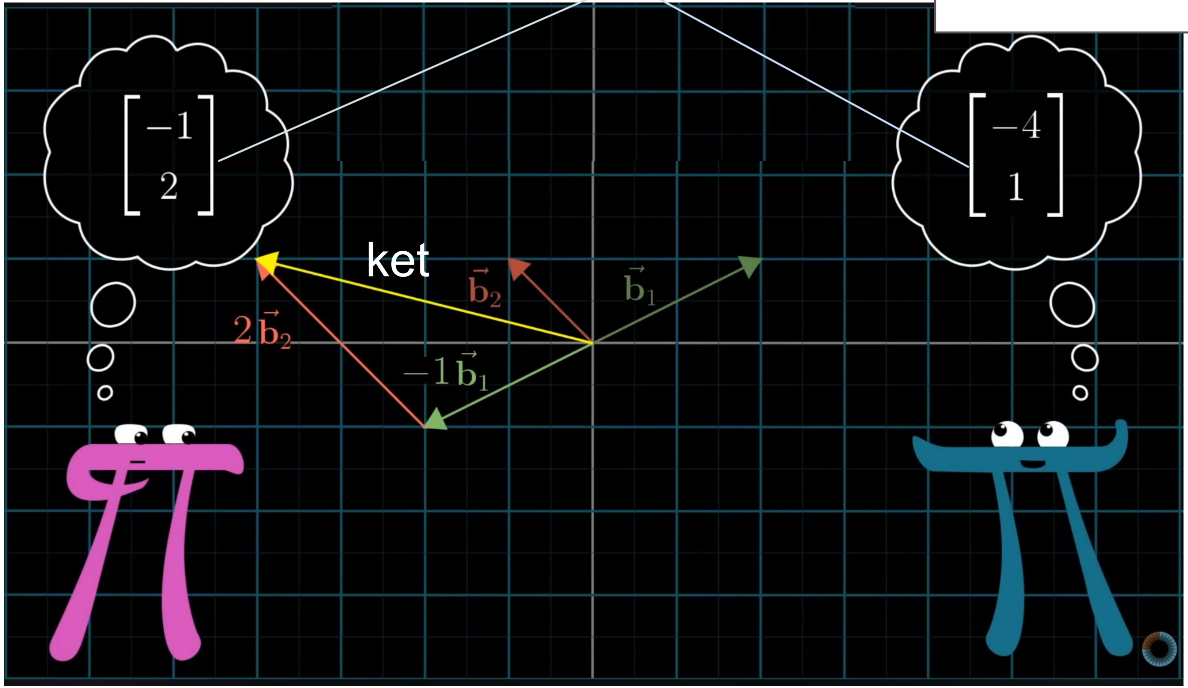


- Examples
  - $\mathbb{R}^n$ and $\mathbb{C}^n$
  - $L^2(\mathbb{R})$, and $\psi(\mathbf{r}) \in L^2(\mathbb{R})$

Dirac Notation: Motivation

- Analogy

Different representations



Example
Ket |nlm>
|1 0 0>
Position representation/ Wave function

$$\varphi_{n=1,l=0,m=0} = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

Dirac Notation

- A ket $|\psi\rangle$ represent a physical state and is an element of an abstract Hilbert space.

- For every ket $|\psi\rangle$ corresponds a bra $\langle\psi|$ such that the inner product is written $\langle\psi|\phi\rangle$

- Properties

$$\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^*$$
$$\langle\varphi|\lambda_1\psi_1 + \lambda_2\psi_2\rangle = \lambda_1\langle\varphi|\psi_1\rangle + \lambda_2\langle\varphi|\psi_2\rangle$$
$$\langle\lambda_1\varphi_1 + \lambda_2\varphi_2|\psi\rangle = \lambda_1^*\langle\varphi_1|\psi\rangle + \lambda_2^*\langle\varphi_2|\psi\rangle$$
$$\langle\psi|\psi\rangle \text{ réel, positif ; nul si et seulement si } |\psi\rangle = 0$$

Complex conjugation

- Linear Operator

$$|\psi'\rangle = A|\psi\rangle$$
$$A(\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle) = \lambda_1 A|\psi_1\rangle + \lambda_2 A|\psi_2\rangle$$

Dirac notation: Representations

Important representations

$$\langle \mathbf{r}|\psi\rangle = \psi(\mathbf{r})$$

$$\langle \mathbf{p}|\psi\rangle = \psi(\mathbf{p})$$

- Given an orthonormal (discrete) basis $\{|u_i\rangle\}$ $\quad \langle u_i|u_j\rangle = \delta_{ij}$

$$\langle u_j|\psi\rangle = c_j$$

- Closure relation $|\psi\rangle = \sum_i c_i|u_i\rangle = \sum_i |u_i\rangle\langle u_i|\psi\rangle = \left(\sum_i |u_i\rangle\langle u_i|\right)|\psi\rangle$

$$\sum_i |u_i\rangle\langle u_i| = \mathbb{1}$$

- Representation of ket, bras and operators

$$A_{ij} = \langle u_i|A|u_j\rangle$$

$$\begin{pmatrix} \langle u_1|\psi\rangle \\ \langle u_2|\psi\rangle \\ \vdots \\ \langle u_i|\psi\rangle \\ \vdots \end{pmatrix} \qquad (\langle\varphi|u_1\rangle\langle\varphi|u_2\rangle\ldots\langle\varphi|u_i\rangle\ldots) \qquad \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1j} & \cdots \\ A_{21} & A_{22} & \cdots & A_{2j} & \cdots \\ \vdots & \vdots & \ddots & \vdots & \ddots \\ A_{i1} & A_{i2} & \cdots & A_{ij} & \cdots \\ \vdots & \vdots & \ddots & \vdots & \ddots \end{pmatrix}$$

Examples

- Projectors onto $|\psi\rangle$ ($\langle\psi|\psi\rangle = 1$)

Hermitian Conjugate

$$P_\psi = |\psi\rangle\langle\psi| \qquad P_\psi|\varphi\rangle = |\psi\rangle\langle\psi|\varphi\rangle \qquad P_\psi^2 = |\psi\rangle\langle\psi| = P_\psi \qquad P_\psi^\dagger = |\psi\rangle\langle\psi| = P_\psi$$

- Closure relation $\sum_i |u_i\rangle\langle u_i| = \mathbb{1}$

$$P_1 + P_2 + P_3 = \mathbb{1}$$

- Change of Basis $\{|u_i\rangle\}$ & $\{|t_k\rangle\}$
  - Change of basis matrix

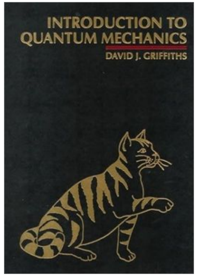
$$S_{ik} = \langle u_i|t_k\rangle$$

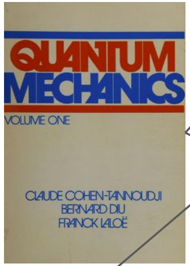
$$\begin{aligned}\langle u_i|\psi\rangle &= \langle u_i|\mathbb{1}|\psi\rangle = \langle u_i|P_{\{t_k\}}|\psi\rangle \\ &= \sum_k \langle u_i|t_k\rangle\langle t_k|\psi\rangle \\ &= \sum_k S_{ik}\langle t_k|\psi\rangle\end{aligned}$$

- Density Operator

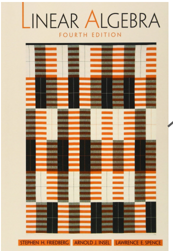
References

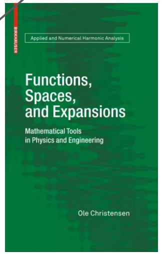
- Quantum mechanics

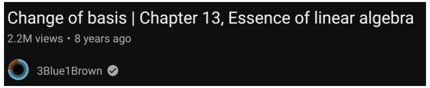




- Linear algebra







Homework

Chapter II: (A, B, C), (D, E)

True & False

Density Operator: Complement E_{III}

Thank you for your attention!