

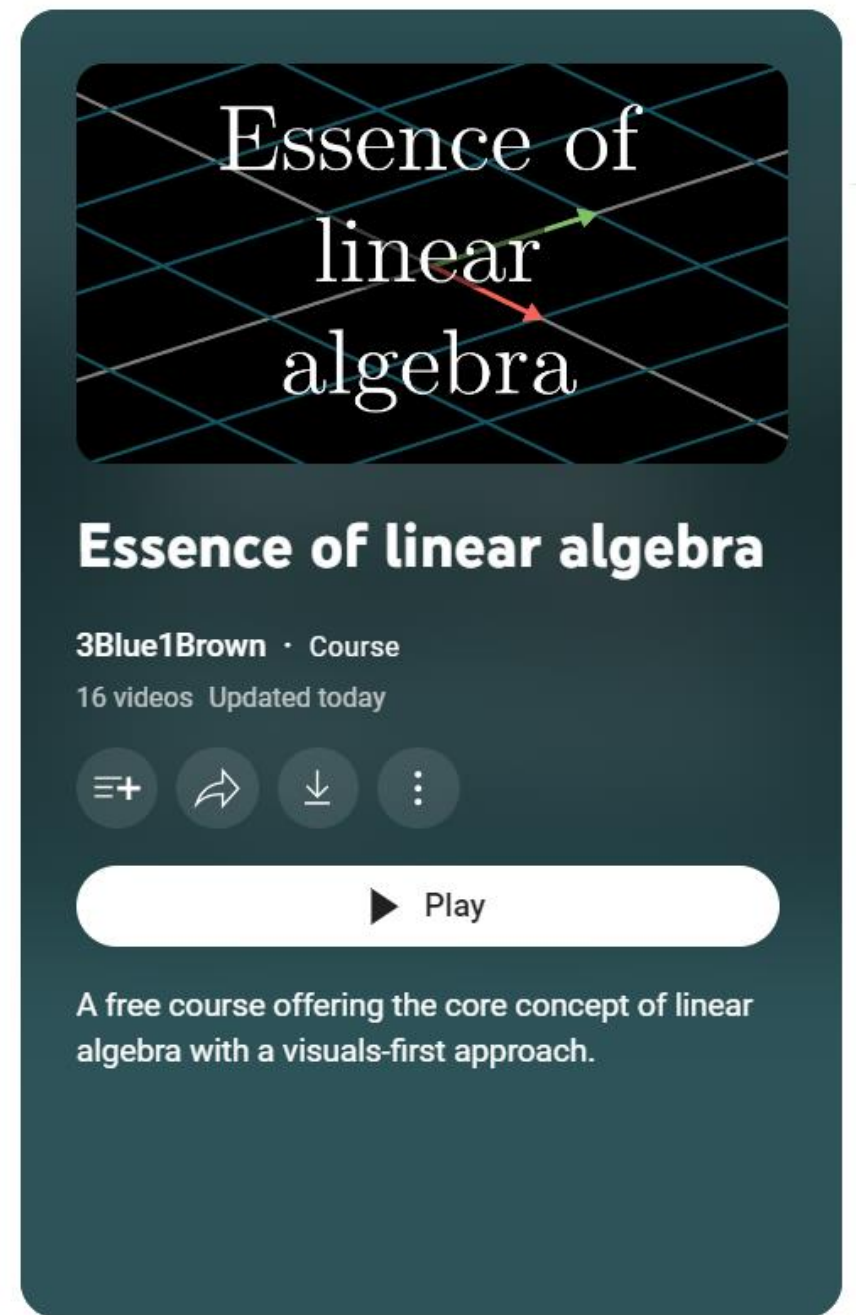


TD2 – Math review

Basic mathematics for quantum mechanics

Basic vector operation

Strongly recommended: Linear algebra course by 3Blue1Brown



Essence of
linear
algebra

Essence of linear algebra

3Blue1Brown · Course

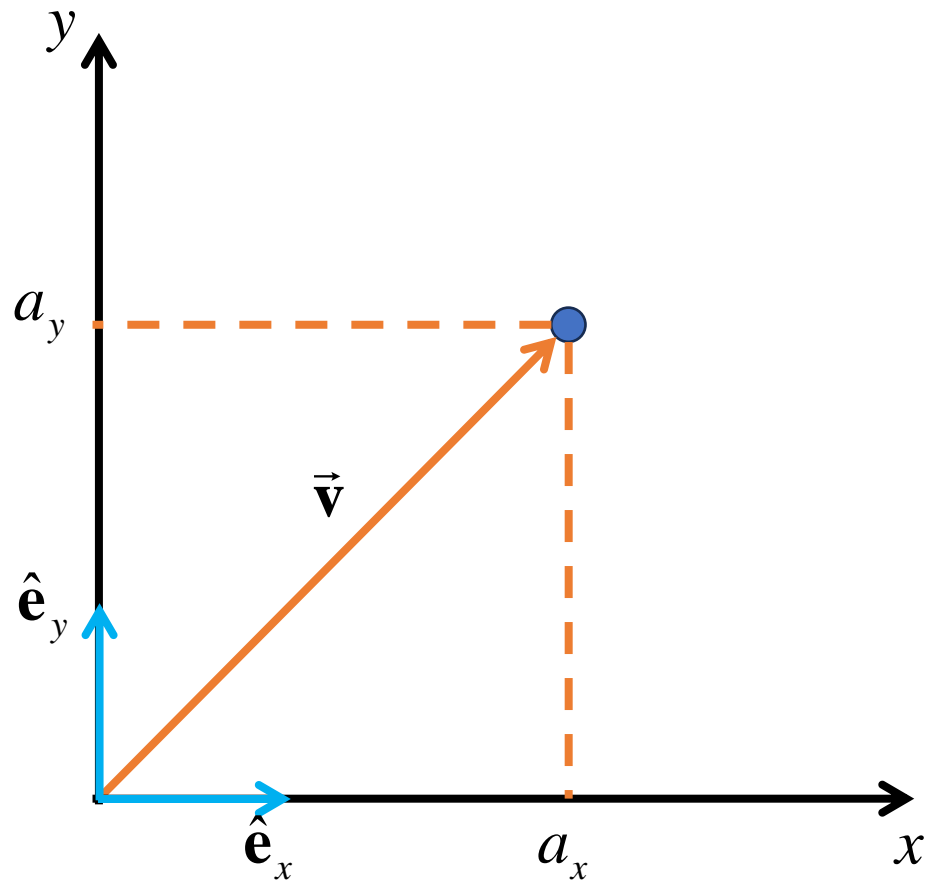
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A free course offering the core concept of linear algebra with a visuals-first approach.

<https://tinyurl.com/3b1bLA>

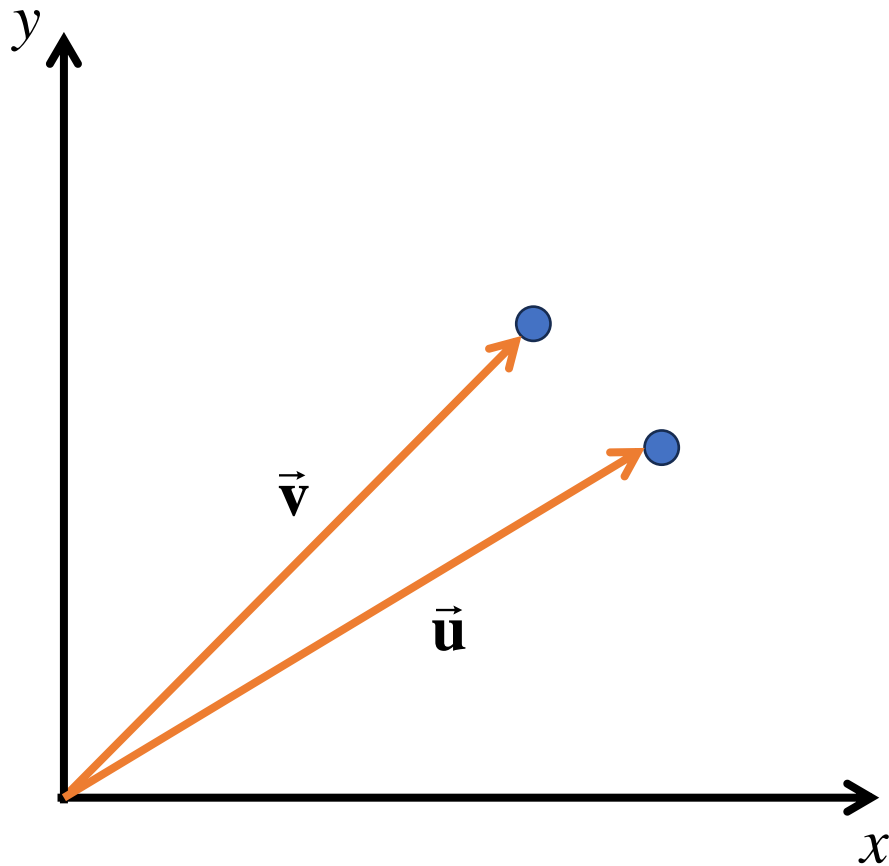


$$\vec{v} = a_x \hat{e}_x + a_y \hat{e}_y$$

$$= \begin{pmatrix} a_x \\ a_y \end{pmatrix}$$

$$\hat{e}_x = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\hat{e}_y = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



$$\vec{\mathbf{v}} = a_x \hat{\mathbf{e}}_x + a_y \hat{\mathbf{e}}_y$$

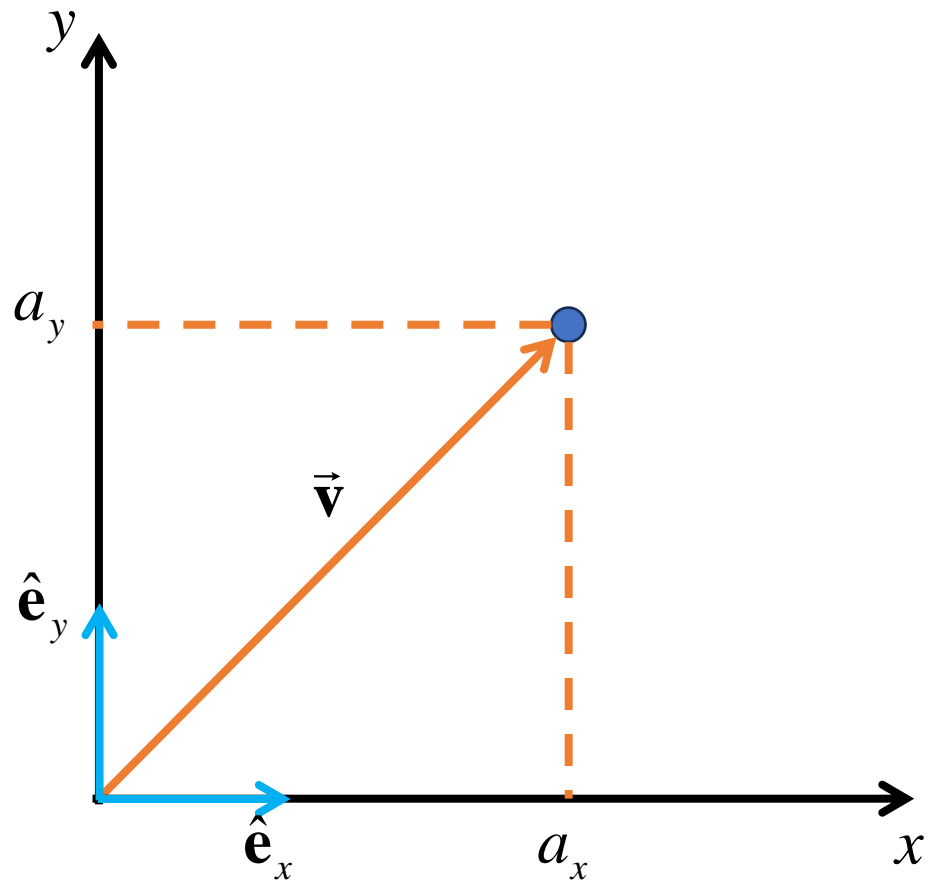
$$\vec{\mathbf{u}} = b_x \hat{\mathbf{e}}_x + b_y \hat{\mathbf{e}}_y$$

Scalar product

$$\vec{\mathbf{v}} \cdot \vec{\mathbf{u}} \equiv a_x b_x + a_y b_y$$

It's a matrix multiplication

$$\vec{\mathbf{v}}^\dagger \cdot \vec{\mathbf{u}} = \begin{pmatrix} a_x & a_y \end{pmatrix} \begin{pmatrix} b_x \\ b_y \end{pmatrix}$$



$$\vec{\mathbf{v}} = a_x \hat{\mathbf{e}}_x + a_y \hat{\mathbf{e}}_y$$

Projection

$$v_x = \hat{\mathbf{e}}_x^\dagger \cdot \vec{\mathbf{v}} = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \end{pmatrix} = a_x$$

$$v_y = \hat{\mathbf{e}}_y^\dagger \cdot \vec{\mathbf{v}} = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \end{pmatrix} = a_y$$

State 2 ————— $E_2, |\varphi_2\rangle$

State 1 ————— $E_1, |\varphi_1\rangle$

Quantum state

$$|\psi\rangle = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle$$
$$= \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

It's analogous to

$$\vec{v} = a_x \hat{e}_x + a_y \hat{e}_y$$
$$= \begin{pmatrix} a_x \\ a_y \end{pmatrix}$$

However, a_1 and a_2 are complex

$$a_n = \alpha + \beta i \quad i^2 = -1$$

State 2 ————— $E_2, |\varphi_2\rangle$

State 1 ————— $E_1, |\varphi_1\rangle$

Quantum state

$$|\psi\rangle = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle$$

$$|\nu\rangle = b_1 |\varphi_1\rangle + b_2 |\varphi_2\rangle$$

Scalar product

$$\langle \psi || \nu \rangle \equiv \langle \psi | \nu \rangle = a_1^* b_1 + a_2^* b_2$$

$$a_1^* = (\alpha + \beta i)^* = \alpha - \beta i$$

It's a matrix multiplication

$$\langle \psi | \nu \rangle = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix} \begin{pmatrix} b_x \\ b_y \end{pmatrix}$$

State 2 ————— $E_2, |\varphi_2\rangle$

State 1 ————— $E_1, |\varphi_1\rangle$

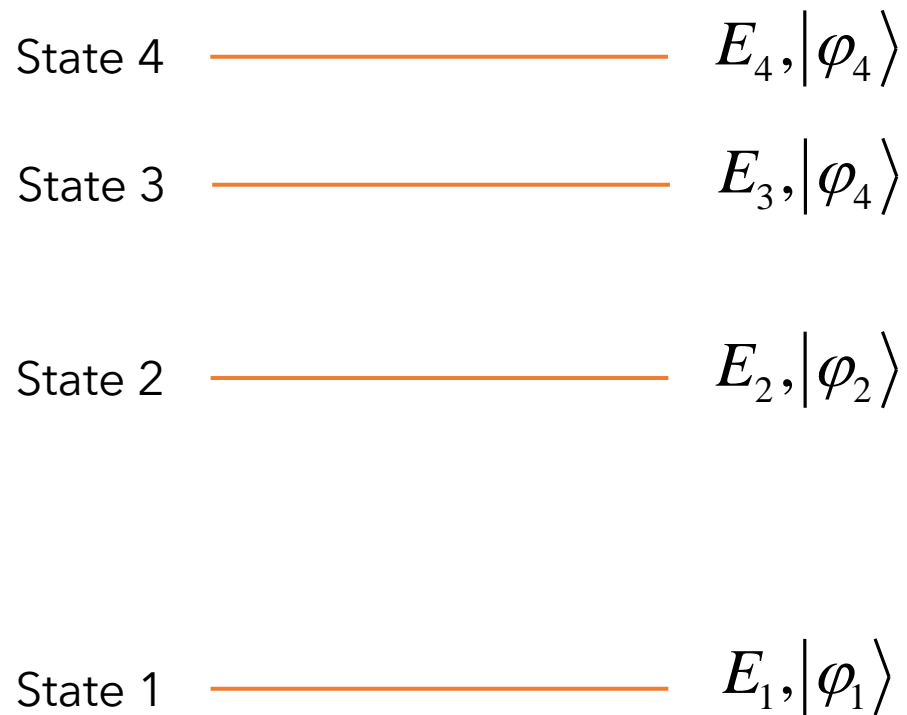
Quantum state

$$|\psi\rangle = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle$$
$$= \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

Projection

$$\langle \varphi_1 | \psi \rangle \equiv \langle \varphi_1 | \psi \rangle$$
$$= \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1$$

$$\langle \varphi_2 | \psi \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_2$$



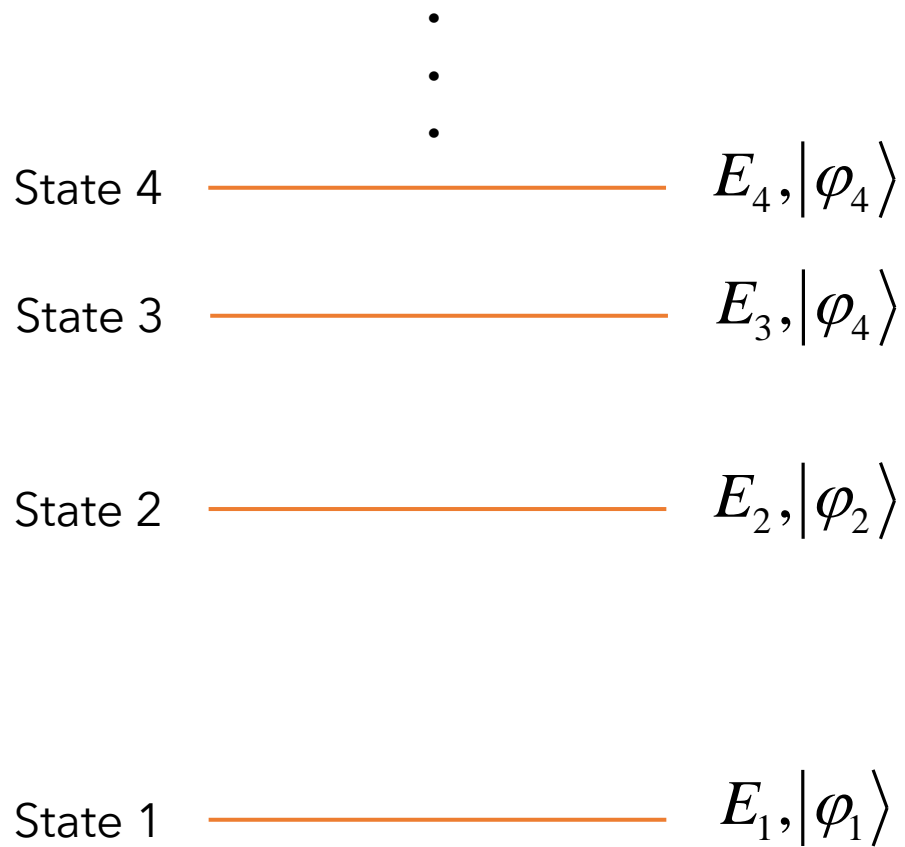
Quantum state

$$|\psi\rangle = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle + a_3 |\varphi_3\rangle + a_4 |\varphi_4\rangle$$

$$= \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

Projection on state 2, for example

$$\langle \varphi_2 | \psi \rangle = (0 \quad 1 \quad 0 \quad 0) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = a_2$$



Quantum state

$$|\psi\rangle = \sum_n a_n |\varphi_n\rangle$$

Projection on state 2, for example

$$\langle\varphi_2|\psi\rangle = \langle\varphi_2|\sum_n a_n |\varphi_n\rangle$$

$$= \sum_n a_n \langle\varphi_2|\varphi_n\rangle$$

$$= \sum_n a_n \delta_{2n} \quad \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$$= 0 + a_2 + 0 + \dots = a_2$$

Ket

$|\psi\rangle$

Bra

$\langle\psi|$

vector

$$|\psi\rangle = (\langle\psi|)^*$$

$$c|\psi\rangle = |\varphi\rangle$$

vector

$$|\psi_1\rangle + |\psi_2\rangle = |\varphi\rangle$$

vector

$$\langle\psi| \times |\varphi\rangle \equiv \langle\psi|\varphi\rangle = c$$

scalar (simple number)

$$|\psi_1\rangle \times |\psi_2\rangle \rightarrow \textit{forbidden!}$$

$$|\varphi\rangle \times \langle\psi| \equiv |\varphi\rangle\langle\psi| = \hat{O}$$

operator

$$\hat{O}|\psi\rangle = |\varphi\rangle$$

vector

Consider

$$|\psi\rangle = \sum_n a_n |\varphi_n\rangle \quad \text{with} \quad \langle \varphi_m | \varphi_n \rangle = \delta_{mn}$$

1. Show that

$$a_m = \langle \varphi_m | \psi \rangle$$

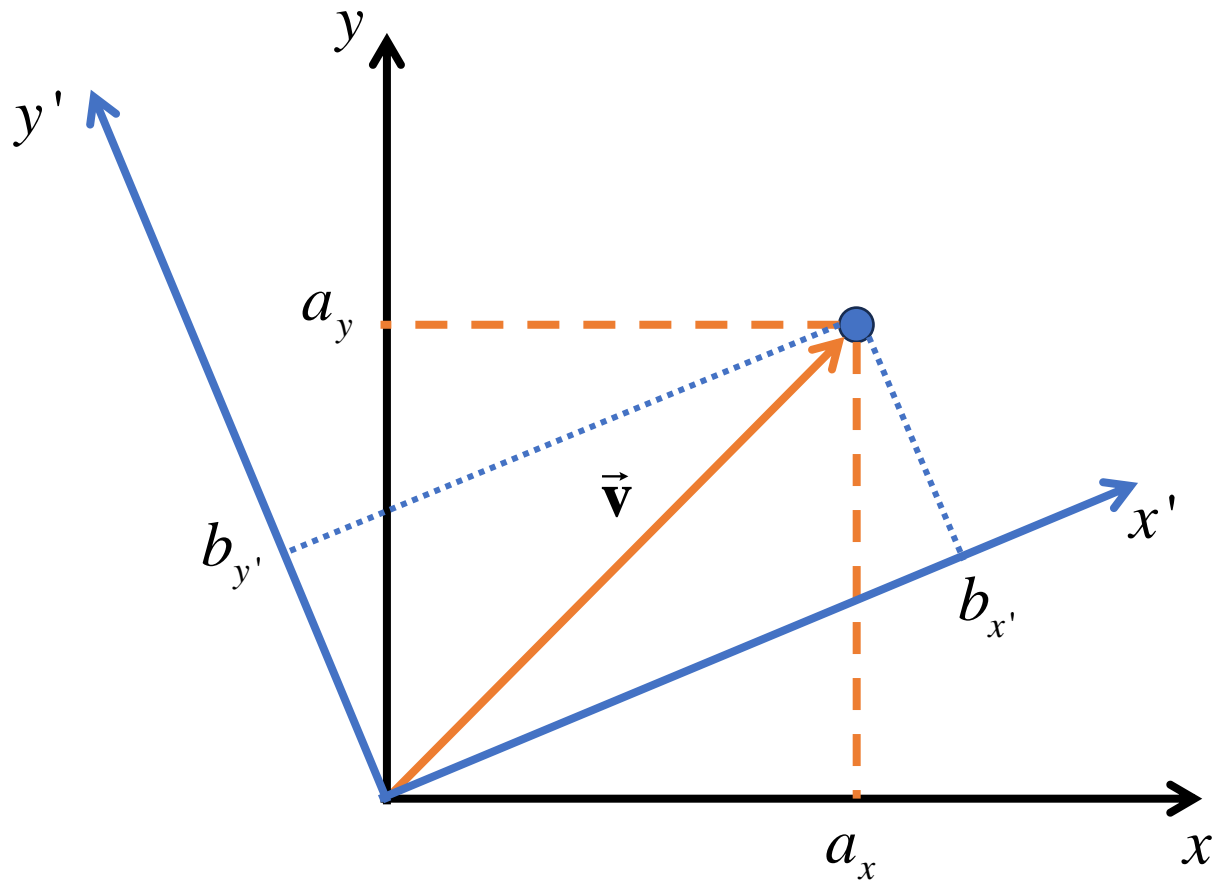
2. Verify that

$$|\psi\rangle = \sum_n |\varphi_n\rangle \langle \varphi_n | \psi \rangle$$

3. Show that

$$\sum_n |\varphi_n\rangle \langle \varphi_n | = \mathbf{1}$$

Basis change



$$\vec{v} = a_x \hat{e}_x + a_y \hat{e}_y$$

$$\vec{v} = b_{x'} \hat{e}_{x'} + b_{y'} \hat{e}_{y'}$$

Consider

$$|\psi\rangle = \sum_n a_n |\varphi_n\rangle$$

Show that this vector is

$$|\psi\rangle = \sum_k b_k |\chi_k\rangle$$

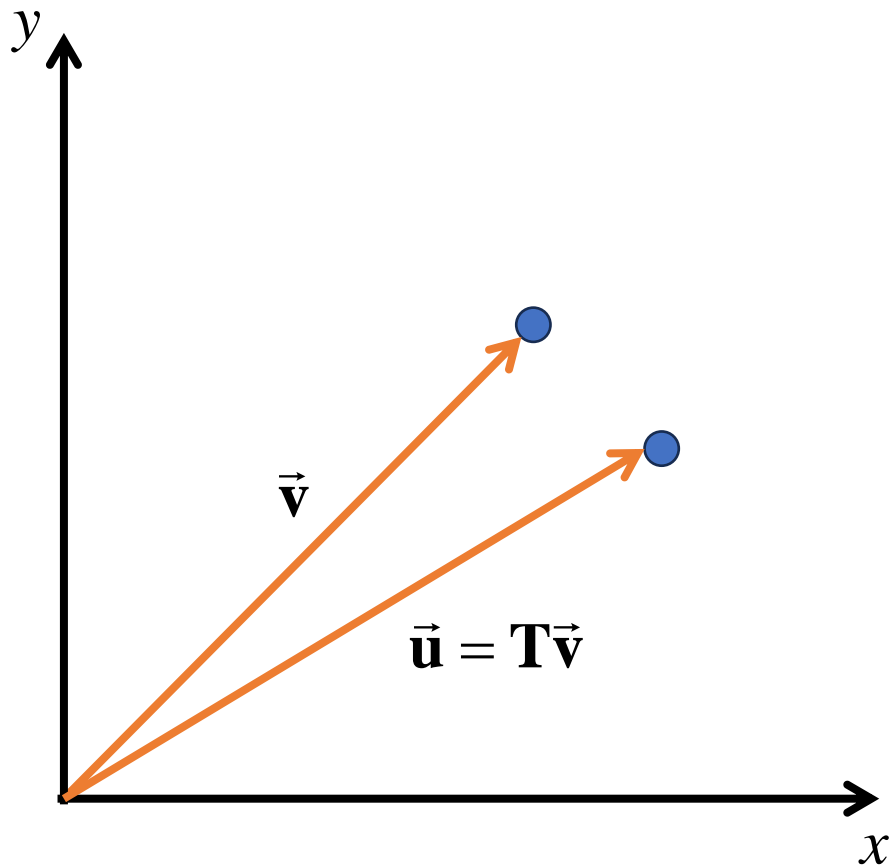
where

$$b_k = \sum_n a_n \langle \chi_k | \varphi_n \rangle$$

Hint: Use

$$\sum_k |\chi_k\rangle \langle \chi_k| = 1$$

Linear transformation



$$\vec{\mathbf{v}} = a_x \hat{\mathbf{e}}_x + a_y \hat{\mathbf{e}}_y$$

$$\mathbf{T} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix}$$

Transformation

$$\mathbf{T}\vec{\mathbf{v}} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} a_x \\ a_y \end{pmatrix}$$

$$= \begin{pmatrix} t_{11}a_x + t_{12}a_y \\ t_{21}a_x + t_{22}a_y \end{pmatrix}$$

$$= \vec{\mathbf{u}}$$

State 2 ————— $E_2, |\varphi_2\rangle$

State 1 ————— $E_1, |\varphi_1\rangle$

Quantum state

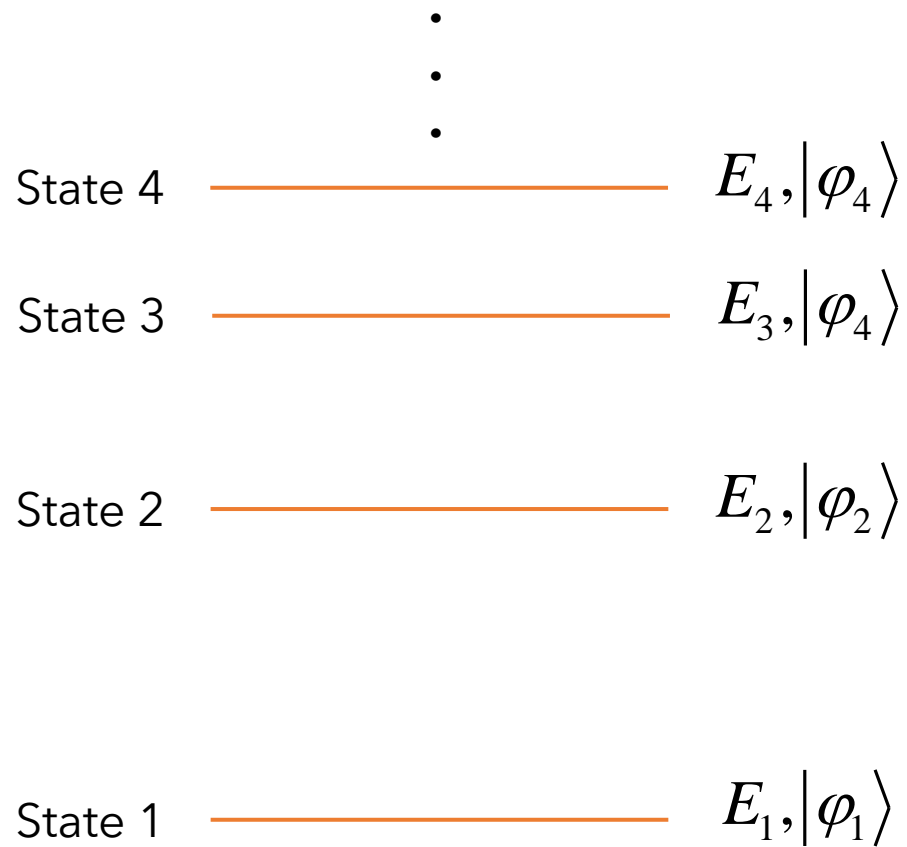
$$|\psi\rangle = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle$$

Operator

$$\hat{O} = \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix}$$

Transformation

$$\begin{aligned} \hat{O}|\psi\rangle &= \begin{pmatrix} O_{11} & O_{12} \\ O_{21} & O_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \\ &= \begin{pmatrix} O_{11}a_1 + O_{12}a_2 \\ O_{21}a_1 + O_{22}a_2 \end{pmatrix} \\ &= |\nu\rangle \end{aligned}$$



Quantum state

$$|\psi\rangle = \sum_n a_n |\varphi_n\rangle$$

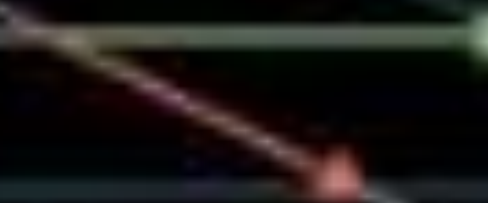
Operation

$$\hat{O}|\psi\rangle = |\nu\rangle$$

The transformation is linear if

$$\hat{O} \sum_n a_n |\varphi_n\rangle = \sum_n a_n \hat{O} |\varphi_n\rangle$$

Linear transformations



Eigenvectors and eigenvalues

Eigenvector



$$\hat{H}|\psi\rangle = E|\psi\rangle$$



Eigenvalue

Eigenvectors

Eigenvalues

$$A\vec{v} = \lambda\vec{v}$$

Continuous spectra

Discrete spectrum (Energy, Spin, ...)

$$\hat{A}|a_m\rangle = a_m|a_m\rangle$$

$$\langle a_m|a_n\rangle = \delta_{mn}$$

$$\sum_n |a_n\rangle\langle a_n| = 1$$

$$|\alpha\rangle = \sum_n |a_n\rangle\langle a_n|\alpha\rangle$$

Continuous spectrum (Position, Momentum, ...)

$$\hat{\xi}|\xi'\rangle = \xi'|\xi'\rangle$$

$$\langle \xi'| \xi'' \rangle = \delta(\xi' - \xi'')$$

$$\int d\xi' |\xi'\rangle\langle \xi'| = 1$$

$$|\alpha\rangle = \int d\xi' |\xi'\rangle\langle \xi'|\alpha\rangle$$

$$|\alpha\rangle = \int d\xi' |\xi'\rangle \langle \xi' | \alpha \rangle$$

$$\alpha(\xi') \equiv \langle \xi' | \alpha \rangle$$

Wave function

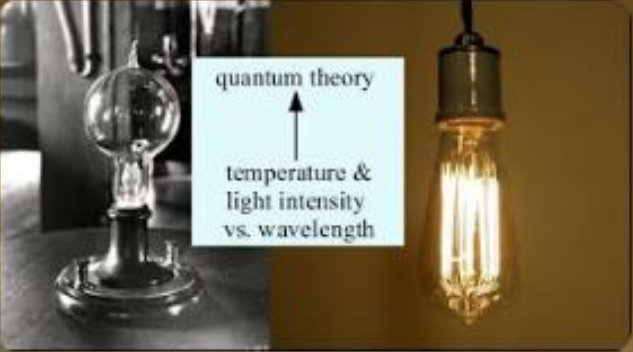
$$|\alpha\rangle = \int d\xi' \alpha(\xi') |\xi'\rangle$$

Example

Position basis $\langle x|\psi\rangle = \psi(x)$ $|\psi\rangle = \int dx \psi(x)|x\rangle$

Momentum basis $\langle p|\psi\rangle = \psi(p)$ $|\psi\rangle = \int dp \psi(p)|p\rangle$

Recommended: Quantum mechanics course by ViaScience



Quantum Mechanics

ViaScience

30 videos 345,216 views Last updated on Jul 17, 2021

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This series draws from several sources, especially from the 1935 text by Pauling and Wilson, *Introduction to Quantum Mechanics*, reprinted by Dover Publications, 1985, ISBN 978-0-486-64871-2; Cohen-Tannoudji, Diu and Laloe, *Quantum Mechanics*, Wiley, 1977, ISBN 0-471-16432-1; and I. N. Levine, *Quantum Chemistry*, 7th ed., Pearson, 2013, ISBN 978-0321803450.

<https://tinyurl.com/viasciQM>

To know more:

Bras and kets

- Sakurai, Modern quantum mechanics, **1994**, Ch 1.

Available for download at:

amubox.univ-amu.fr/s/xXAiMZrDPb9RMRX

Ask me for the password.

For TP2 next week (9 Oct):

- Bring a list of 5 references you think are important for your topic review
- Vijay and I be there to discuss your topic. Come with questions!