

Physical Chemistry III

2022.03.21

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- Schrödinger equation – History
- Bra-ket notation
- Particle in a box

Quantum Physics for Poets (시인을 위 한 양자물리학)



Book by Christopher T. Hill
and Leon M. Lederman

10/10
알라딘

10/10
교보문고

4/5
고객센터 - 옥션

Did you like this book?



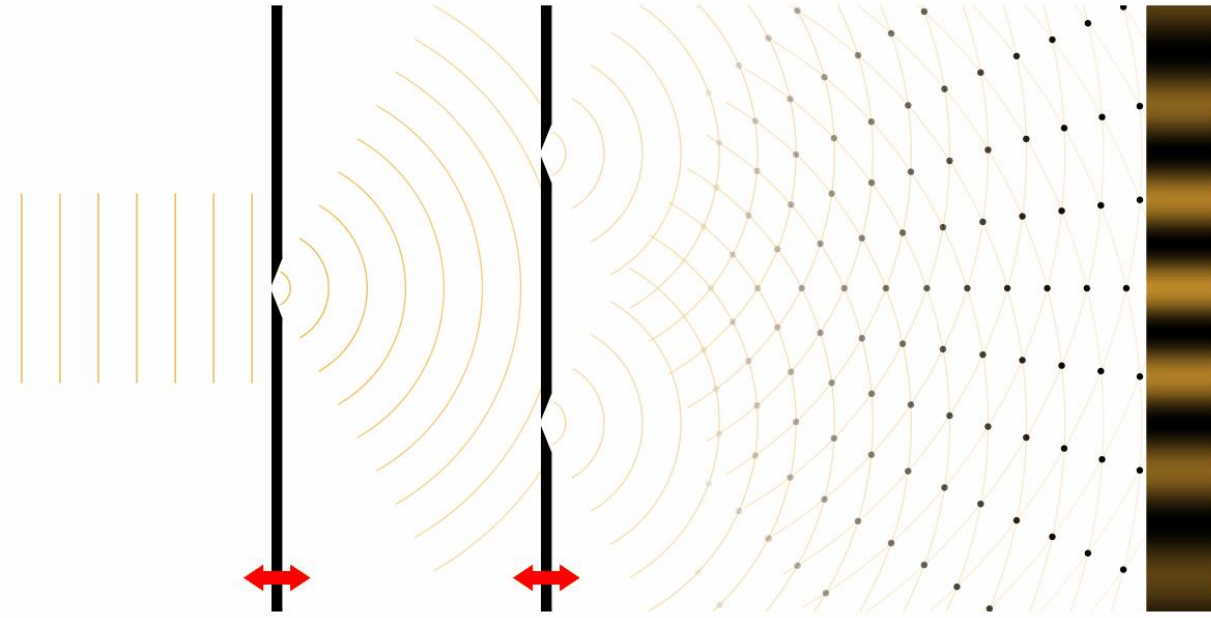
The Times Literary Supplement called their previous book, *Symmetry and the Beautiful Universe*: [A] tour de force of physics made simple. Quantum theory is the bedrock of contemporary physics and the basis of understanding matter in its tiniest dimensions and the vast universe as a whole. ... [Google Books](#)

Originally published: September 11, 2010

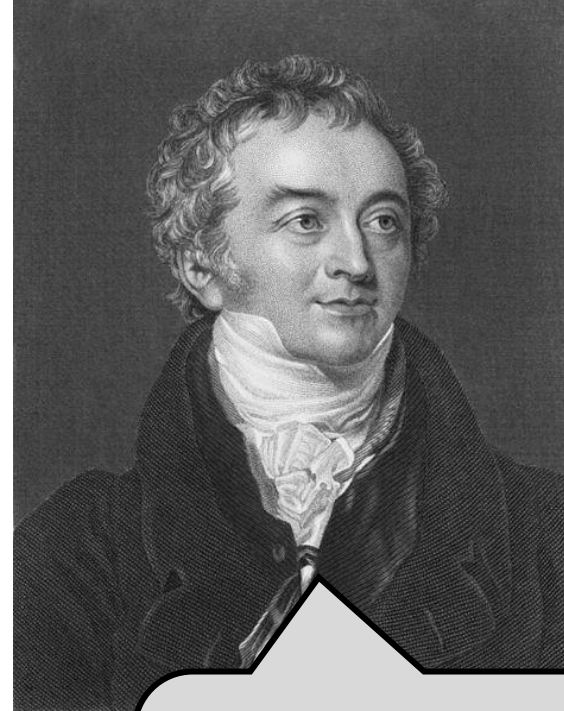
Authors: [Christopher T. Hill](#), [Leon M. Lederman](#)

Double slit experiment

In 1801, Thomas Young



https://javalab.org/en/youngs_double_slit_en/



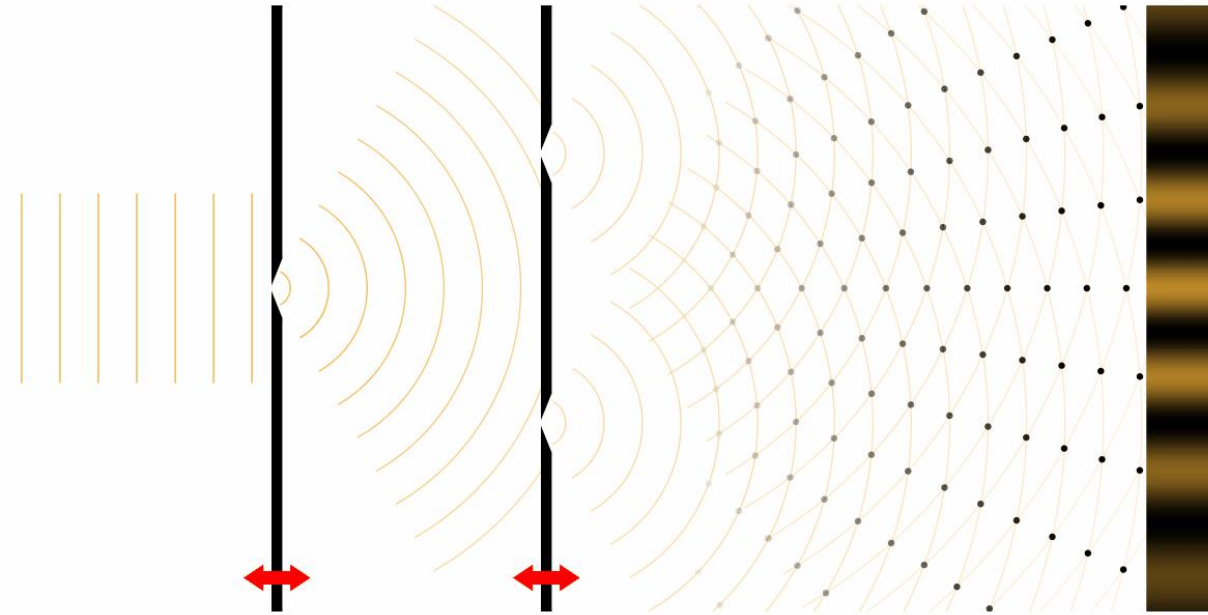
Light is made up
of small discrete
particles!



No. You wrong.
Light is **wave**.

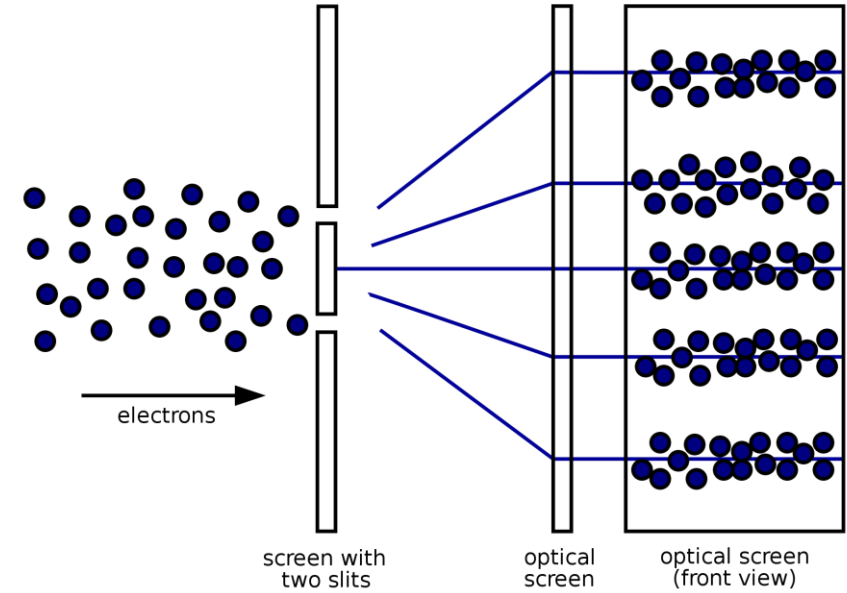
Double slit experiment

In 1801, Thomas Young



https://javalab.org/en/youngs_double_slit_en/

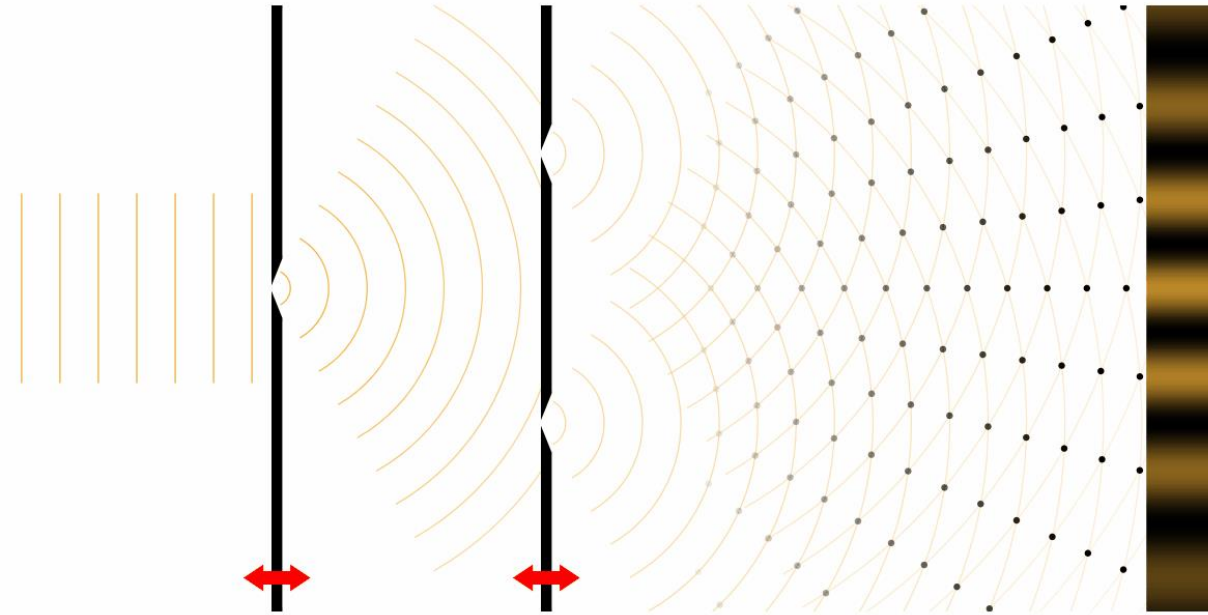
In 1927 at Bell Labs, Clinton Davisson and Lester Germer



Electron is **wave**..?

Double slit experiment

In 1801, Thomas Young



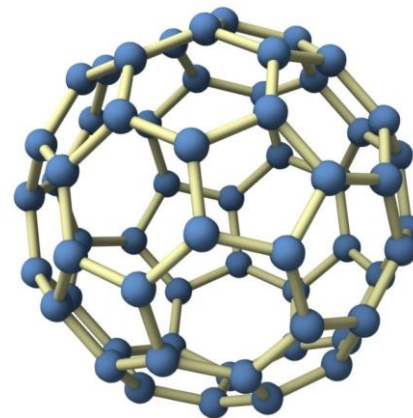
https://javalab.org/en/youngs_double_slit_en/

letters to nature

Wave–particle duality of C_{60} molecules

Markus Arndt, Olaf Nairz, Julian Vos-Andreae, Claudia Keller,
Gerbrand van der Zouw & Anton Zeilinger

*Institut für Experimentalphysik, Universität Wien, Boltzmannngasse 5,
A-1090 Wien, Austria*



Am I **wave**?

Matter wave

In 1924, De Broglie (Ph.D student)



De Broglie hypothesis

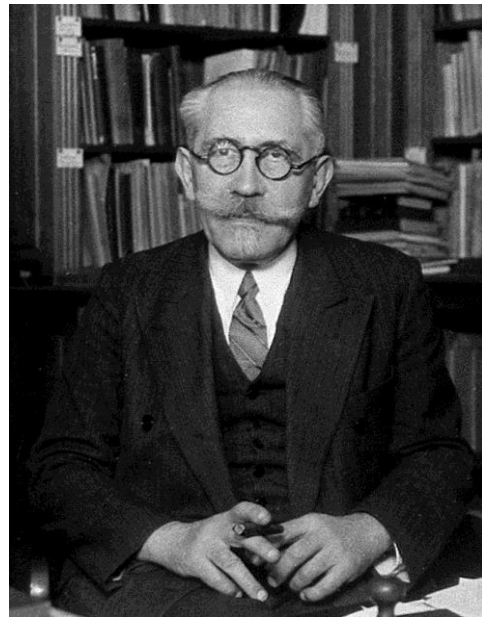
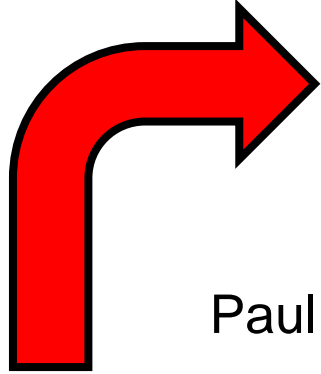
$$\lambda = \frac{h}{p}$$

λ : wavelength of matter wave

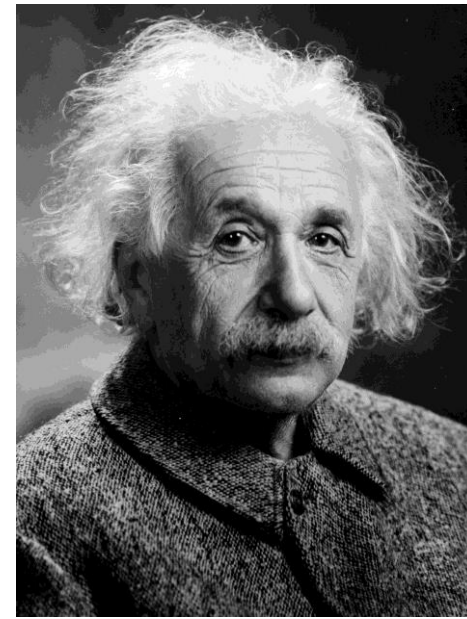
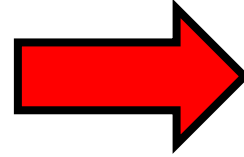
h : Planck constant

p : momentum

Matter wave

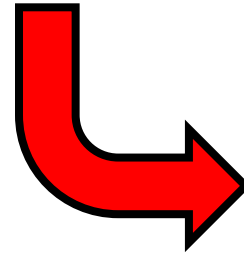


Paul Langevin (Professor of Broglie)



Albert Einstein (Friend of Langevin)

De Broglie (Ph.D student)



Erwin Schrödinger (Research assistant of Einstein)

Schrödinger Equation

In 1925, (published in 1926)



If De Broglie hypothesis is correct,
then it can be described by

Hamiltonian mechanics!

(a.k.a. King of classical mechanics)

$$\hat{H}|\psi\rangle = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0\right)|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle = E|\psi\rangle$$

It is clear!

But I don't know the meaning of $|\psi\rangle$

After Schrödinger Equation

In 1926,



Werner Heisenberg

Uncertainty principle

$$\Delta r \Delta p \geq h$$

$|\psi|^2$ = Probability
density function!



Max Born

After Schrödinger Equation

In 1927 Brussels conference..

Erwin Schrödinger

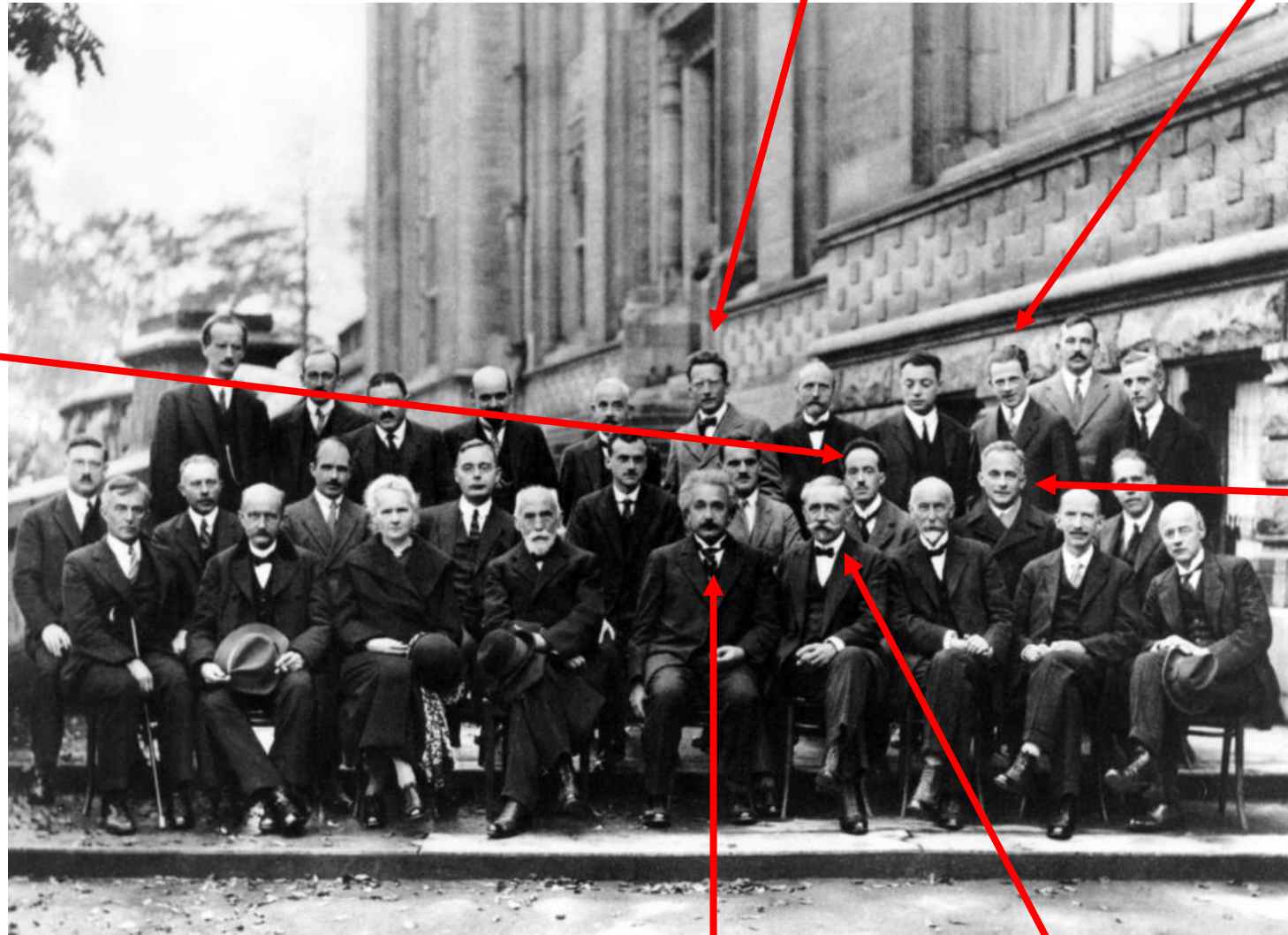
Werner Heisenberg

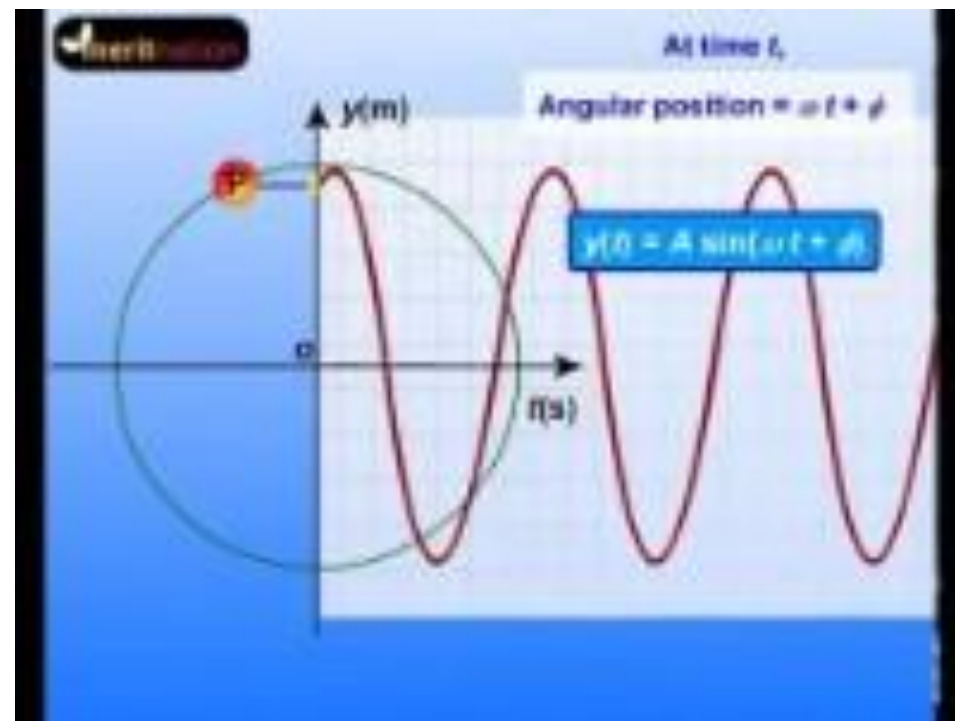
De Broglie

Max Born

Albert Einstein

Paul Langevin



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

Let, $|\psi\rangle = a_1|\varphi_1\rangle + a_2|\varphi_2\rangle + a_3|\varphi_3\rangle$

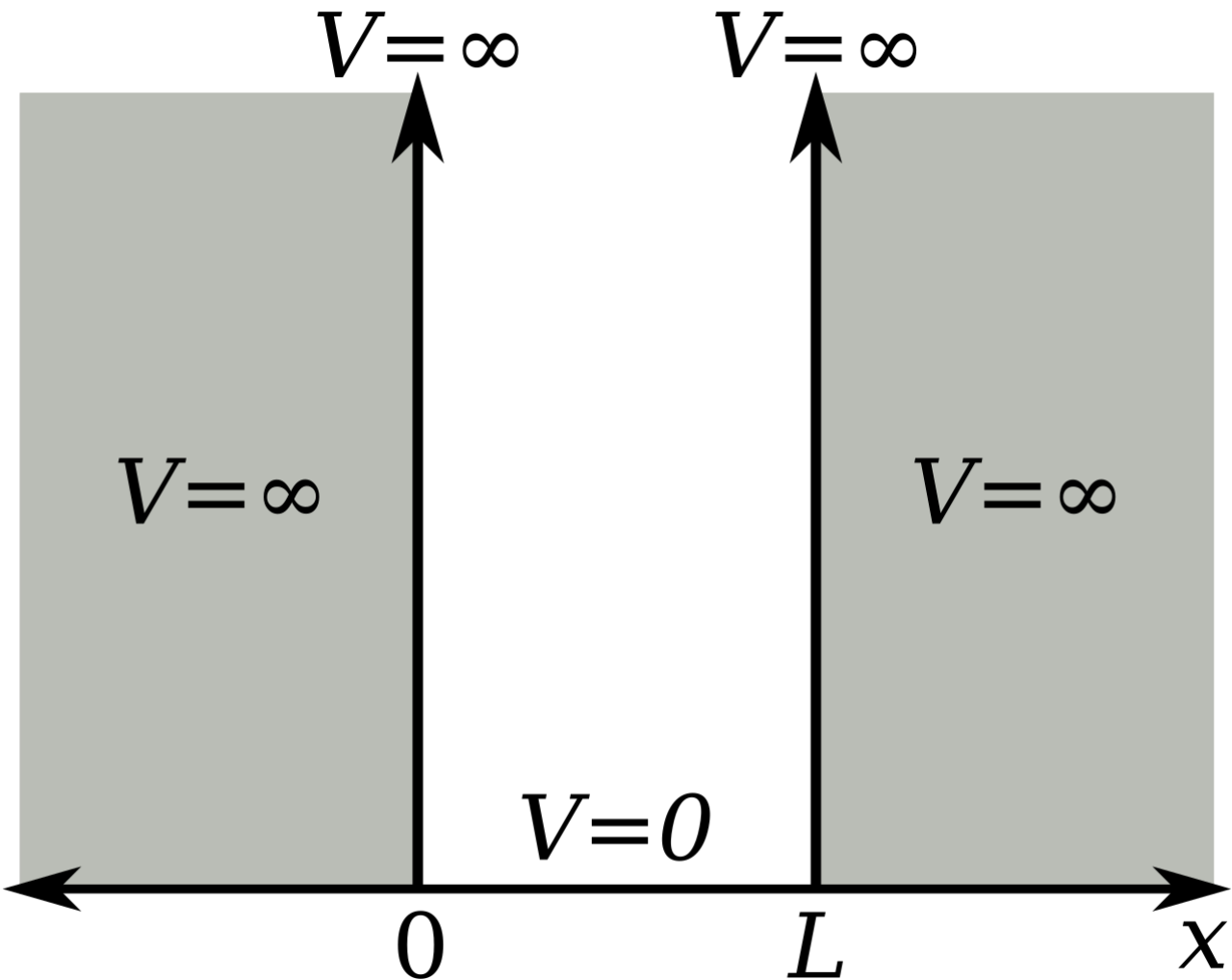
$$|\varphi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |\varphi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |\varphi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \text{Orthonormal basis}$$

$$|\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \quad a_1^2 + a_2^2 + a_3^2 = 1 \quad \langle\varphi_1| = |\varphi_1\rangle^\dagger = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^\dagger = (1 \quad 0 \quad 0)$$

$$\langle\varphi_1|\psi\rangle = (1 \quad 0 \quad 0) \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = a_1: \text{component(weight factor) of } |\varphi_1\rangle$$

$$|\psi\rangle = \sum_{i=1}^3 a_i |\varphi_i\rangle = \sum_{i=1}^3 |\varphi_i\rangle \langle\varphi_i|\psi\rangle = \mathbf{I}|\psi\rangle$$

Particle in a box



$$\hat{H}\psi(x) = E\psi(x)$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{otherwise} \end{cases}$$

$$\psi(x) = \sum_{n=1}^{\infty} a_n \psi_n(x)$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), E_n = \frac{h^2}{8mL^2} n^2$$

[https://github.com/thereexist/Physical_chemistry_3/blob/main/Particle in a box/particle in a box.ipynb](https://github.com/thereexist/Physical_chemistry_3/blob/main/Particle%20in%20a%20box/particle%20in%20a%20box.ipynb)