Applied Quantum Mechanics

Prof. F. Grillot

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Syllabus

Class Times and Location: Monday & Wednesday 8-10 AM (Boelter 9436)

Instructor: Prof. F. Grillot

email: fgrillot@seas.ucla.edu

Office Hours: Tuesday & Thursday 10-11 AM (66-144 Engr. IV.)

Course Website: https://eeweb.ee.ucla.edu

Please make sure your email is entered on the eeweb website in order to receive course email

Midterm: Tuesday November 22, [open book], Wednesday, November 22, 2017, 11AM-12:50PM

Final: Oral presentation based on a research paper, (December)

Syllabus

Grading policy: HW (19%),

Midterm (40%) + Finale Presentation (40%),

Survey (1%)

There will be 4 HWs assigned, typically due every 2-3 weeks in class. Instructor reserves the right to use his judgment rather than strict formulae when determining final grades.

Main Topics (tentative)

Postulates, Schrödinger equation, Fourier transform, Ehrenfest's theorem, Hilbert Space, Observable, Commutation, Infinite well, Bound and Scattering States, Finite Well, Asymmetric double well potential, Tunneling effect, Chemical bond, Stability of Matter, Wave-packet, Quantum harmonic oscillator, Photon polarization, Stern and Gerlach experiment,…

Syllabus

Main Topics (continued)
Angular momentum and spin, Bell's theorem, Entanglement, Perturbation theory, Central force problem, Hydrogen atom, Fermi golden rule, Field quantization, Fermions & bosons, indiscernibility, Krönig-Penney's model, Nonlinear chaotic dynamics in quantum systems.

The exact choice and order of coverage may be adjusted or enhanced during the course

The course will also give various applications of quantum mechanics in our daily life
Telecommunications (Laser), Microelectronics (Nanotransistor)
Medicine (Nuclear Magnetic Resonance)
Microscopy (STM)
Quantum cryptography
Astrophysics (oscillation of nucleons)
Spintronics (Magnetic Hard Drives, RAMs)

Resources

I do not plan to follow a specific textbook. The lectures will present complementary viewpoints and topics. However the following references can be considered to grab more information.

[1] D. J. Griffiths, Introduction to Quantum Mechanics,

[2] R. Liboff, Introductory Quantum Mechanics

[3] P. L. Hagelstein, S. D. Senturia, and T. P. Orlando, Introductory Applied Quantum & Statistical Mechanics

[4] R. P. Feynman, The Feynman Lectures on Physics, Volume III: Quantum Mechanics

[5] C. Cohen-Tannoudji, B. Diu, and F. Laloe, Quantum Mechanics

[6] J. J. Sakurai, Modern Quantum Mechanics

Motivations

Why do we teach quantum mechanics?

A conceptual revolution: a particle can be a wave and a corpuscle (wave-particle duality) !

Quantum mechanics unveils a fundamental theory in physics as the relativity does too

Quantum mechanics fundamentally challenges the rules of all logic e.g. position, measurement, is that real world?

A technological revolution, more than 50% of the gross domestic product is driven by quantum mechanics related technologies (electronics, optoelectronics, nuclear science, lasers, medicine,…)

Directions

Starting point

Interferences with particles of matter, tunneling effect

Thought experiments

Mathematical tools

Probability distribution

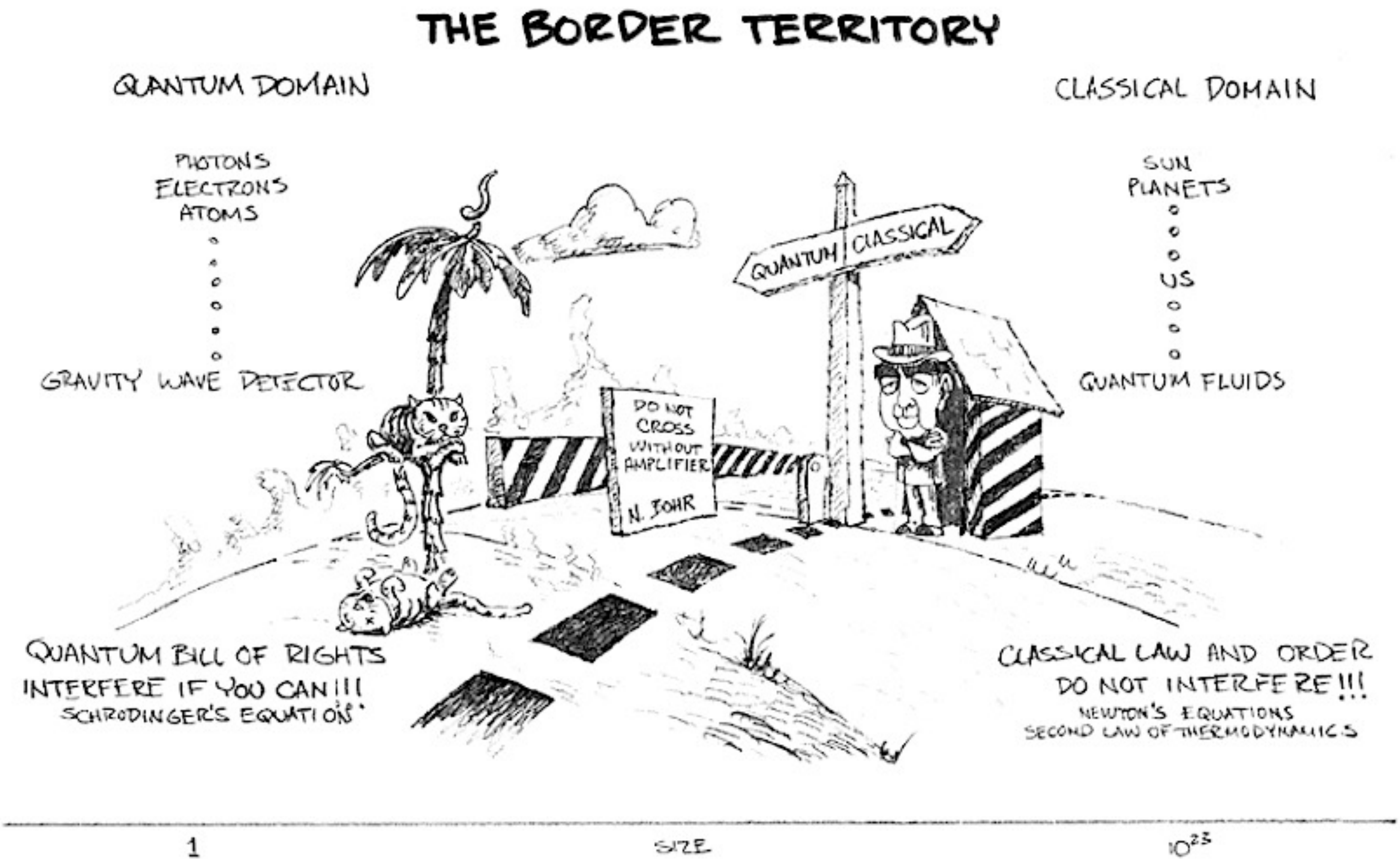
Fourier transform

Linear algebra

Outcomes

Explain the stability of matter, the chemical bond, etc.

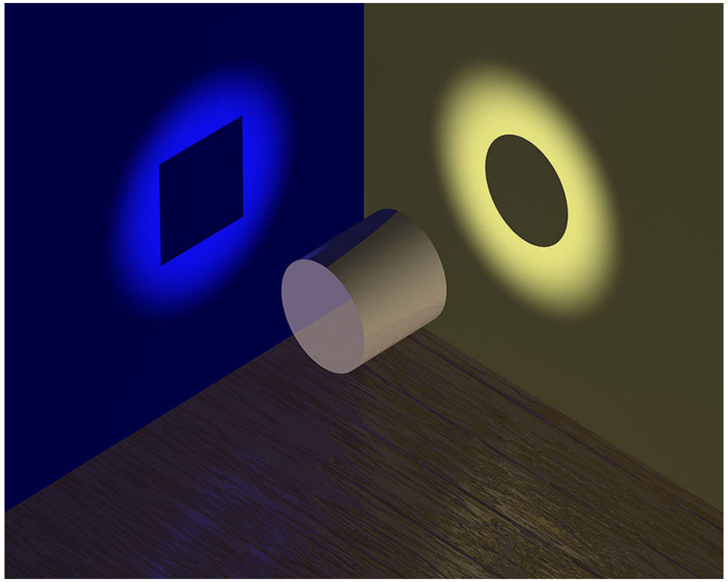
Show various examples of applications of quantum mechanics in our daily life


THE BORDER TERRITORY
QUANTUM DOMAIN
CLASSICAL DOMAIN
PHOTONS
ELECTRONS
ATOMS
GRAVITY WAVE DETECTOR
SUN
PLANETS
US
QUANTUM FLUIDS
QUANTUM | CLASSICAL
DO NOT CROSS WITHOUT AMPLIFIER
N. BOHR
QUANTUM BILL OF RIGHTS
INTERFERE IF YOU CAN!!!
SCHRODINGER'S EQUATION
CLASSICAL LAW AND ORDER
DO NOT INTERFERE!!!
NEWTON'S EQUATIONS
SECOND LAW OF THERMODYNAMICS
1
SIZE
10^23

Section 1

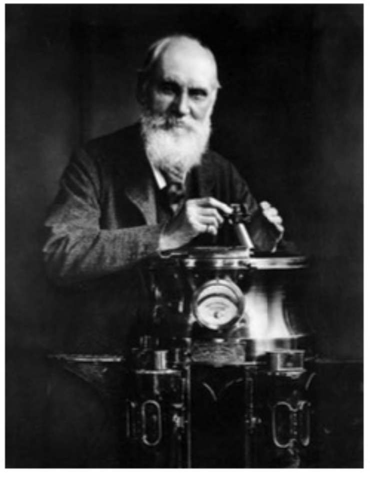
Wave or corpuscle?

The free quantum particle



1.

From Lord Kelvin's clouds to Louis de Broglie's waves



Lord Kelvin (1824-1907)

Louis de Broglie (1892-1987)

Lord Kelvin's clouds

On Friday, April 27, 1900, the British physicist Lord Kelvin said: "*The beauty and clearness of the dynamical theory, which asserts heat and light to be modes of motion, is at present obscured by two clouds*"

What are the clouds?

Lord Kelvin's clouds

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1. The inability to detect the luminous ether, specifically the failure of the Michelson-Morley experiments

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2. The black body radiation effect known as the ultraviolet catastrophe

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1. The inability to detect the luminous ether, specifically the failure of the Michelson-Morley experiments

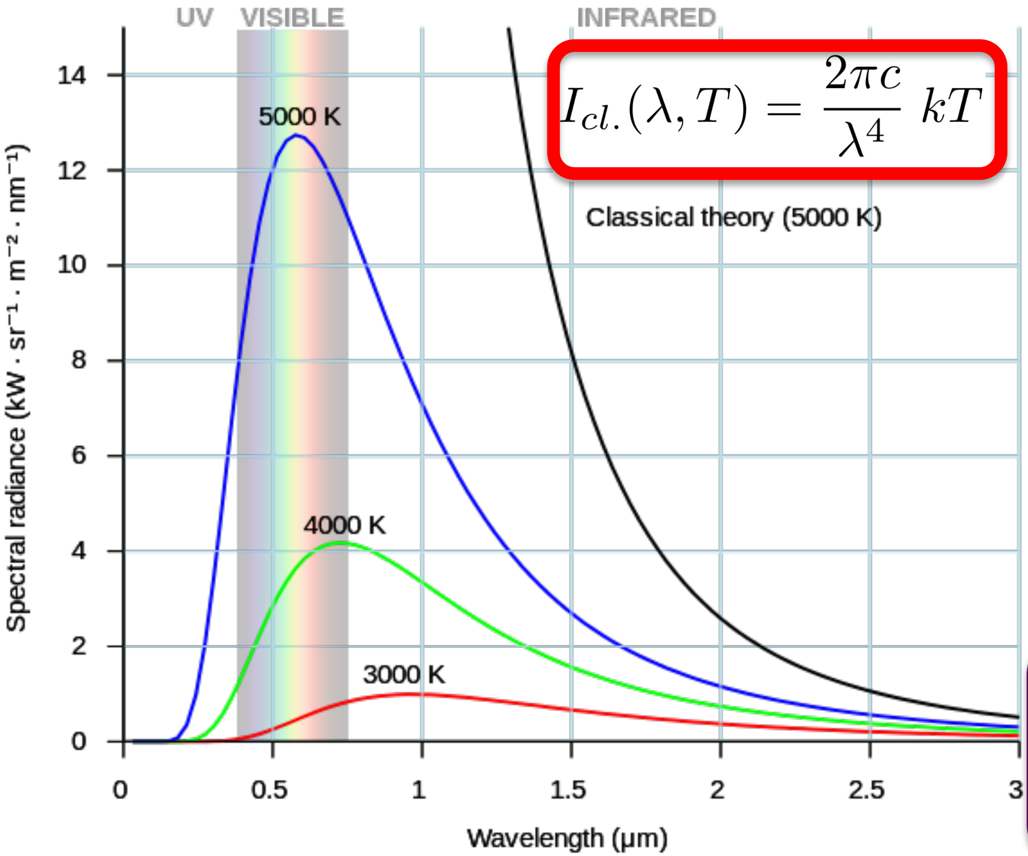
→ theory of the relativity without concept of absolute time

2. The black body radiation effect known as the ultraviolet catastrophe

→ quantum mechanics without concept of universal determinism

Blackbody radiation

Classical physics can be used to describe the intensity of blackbody radiation as a function of frequency for a fixed temperature. This is the so-called Rayleigh-Jeans 's law!



$$\boxed{I_{cl.}(\lambda, T) = \frac{2\pi c}{\lambda^4}\, kT}$$

The equation works for low frequencies, but totally diverges for high frequencies

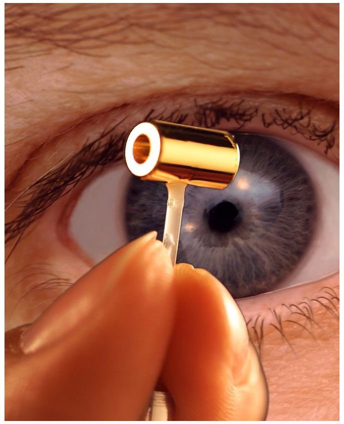
→ ultraviolet catastrophe

Planck's law

$$\boxed{I_{Planck}(\lambda, T) = \frac{2\pi h c^2}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1}}$$

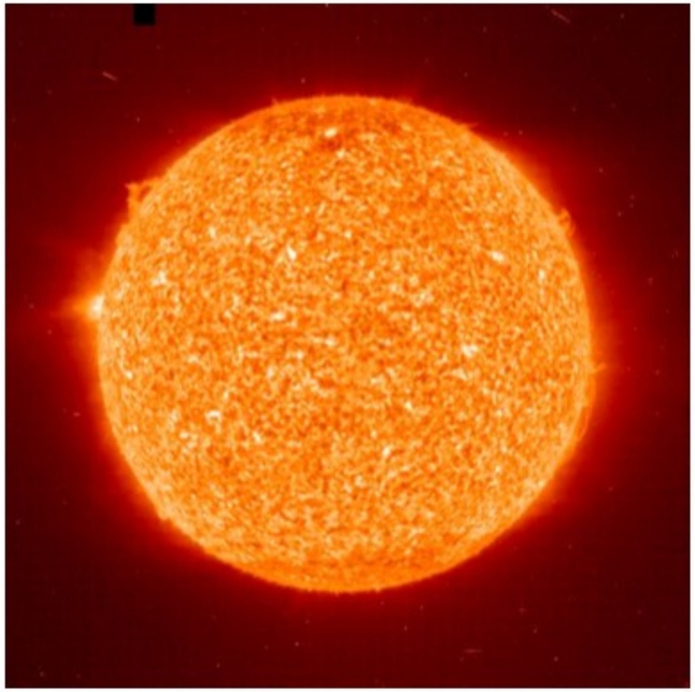
Blackbody radiation

Blackbody radiation is the thermal electromagnetic radiation within or surrounding a body in thermodynamic equilibrium with its environment, or emitted by a black body that is an idealized object absorbing all frequencies (*e.g. hohlraum in German*)



Human body

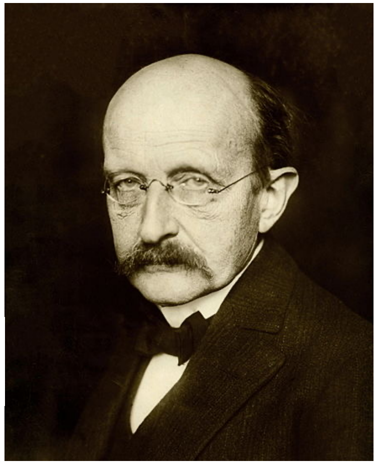
Surface of the sun



Planck's postulate (1900)

The Planck's postulate stands that the energies of the oscillations of electrons which give rise to the radiation must be proportional to integral multiples of the frequency

1918



$$\Delta E = nh\nu = n\hbar\omega \qquad \omega = 2\pi\,\nu$$

Planck's constant

$$h \simeq 6.63\ 10^{-34}\text{Js}$$

Modified Planck's constant

$$\hbar = \frac{h}{2\pi} \simeq 1.05\ 10^{-34}\text{Js}$$

The postulate was introduced in his derivation of his law of black body radiation in 1900. Planck was unable to justify this assumption based on classical physics; he considered quantization as being purely a mathematical trick!

Albert Einstein (1905)

Assuming a light of pulsation ω and momentum k, the quantum of particle named « photon* » by Lewis in 1926 holds an energy and impulsion defined such as:


1921

$$E = \hbar\omega \qquad \vec{p} = \hbar\vec{k} \qquad |\vec{k}| = \frac{2\pi}{\lambda}$$

photon* = Lichtquantum in German

Einstein introduces the concept of light quantization

Is the photon granularity in contradiction with the standard wave equation which should be continuous (Maxwell)?

How to understand the duality nature of Light? (e.g. Light has both properties of wave and particle at the same time).

Does the duality still exist for particles of matter (electrons, etc.)?

Louis de Broglie (1923)

With every particle of matter with mass m and velocity v, a real wave must be associated, related to the momentum by the equation

$$\vec{k} = \frac{\vec{p}}{\hbar}$$

In wavelength,

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p}$$

or even

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

1929

"The fact that, following Einstein's introduction of photons in light waves, one knew that light contains particles which are concentrations of energy incorporated into the wave, suggests that all particles, like the electron, must be transported by a wave into which it is incorporated..."

"My essential idea was to extend to all particles the coexistence of waves and particles discovered by Einstein in 1905 in the case of light and photons"

2.

Waves of matter and interferences

Electron scattering, 1927

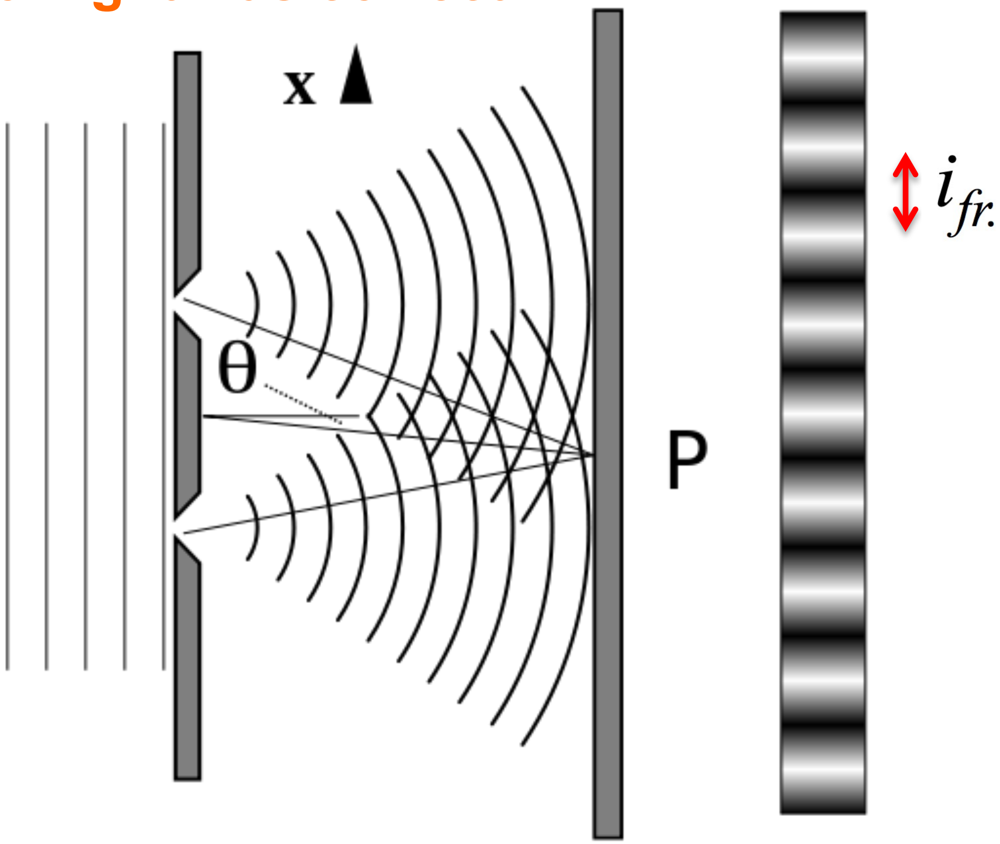
Davisson & Germer

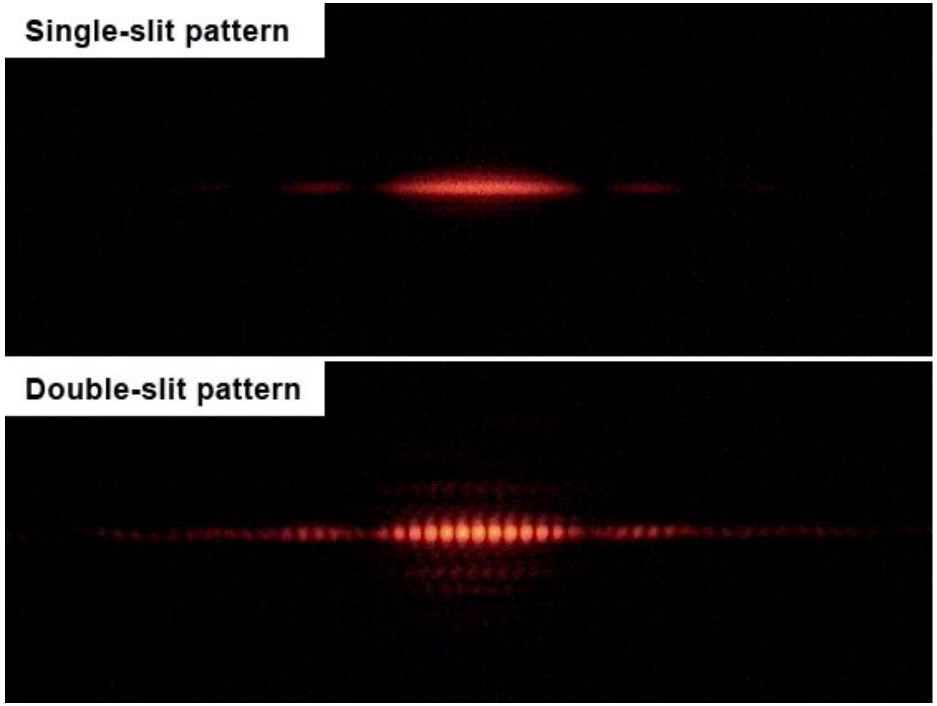
George Thomson

1937

Young's double slit experiments (1801)

The original double-slit experiment in 1801 (well before quantum mechanics). Young thought to have demonstrated that the wave theory of light was correct





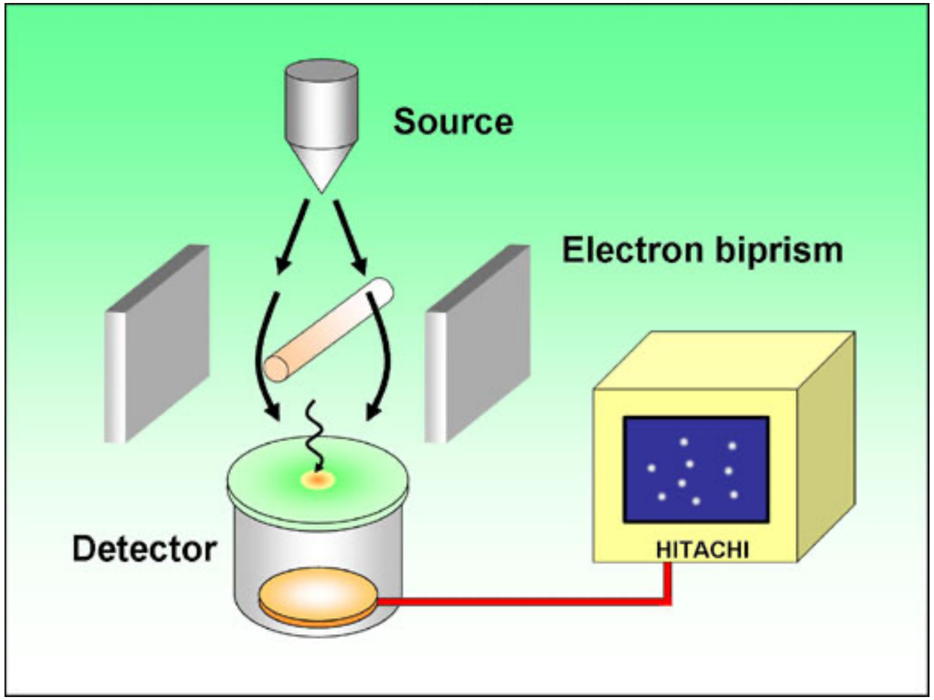
$$i_{fr.} = \frac{\lambda D}{a}$$

Single slit : diffraction pattern

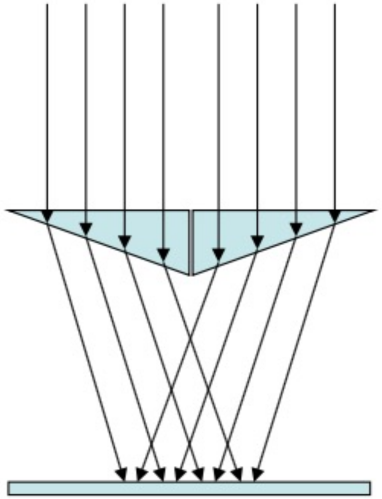
Double slit : diffraction pattern and interference fringes

Double slit experiment with electrons

Electrons are accelerated to 50 kV, with a speed of about 120,000 km/s e.g. 0.4 $\times$ c (~ 10 electrons per second)

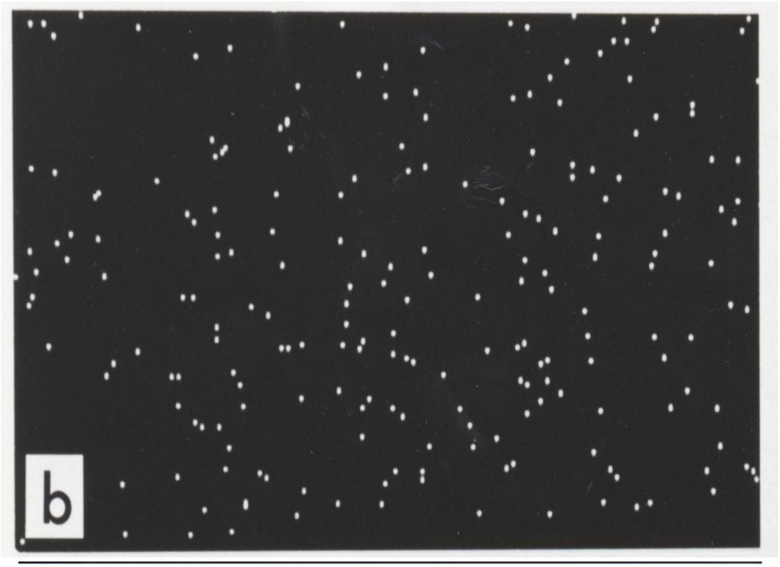


Similar to Fresnel's biprism experiment



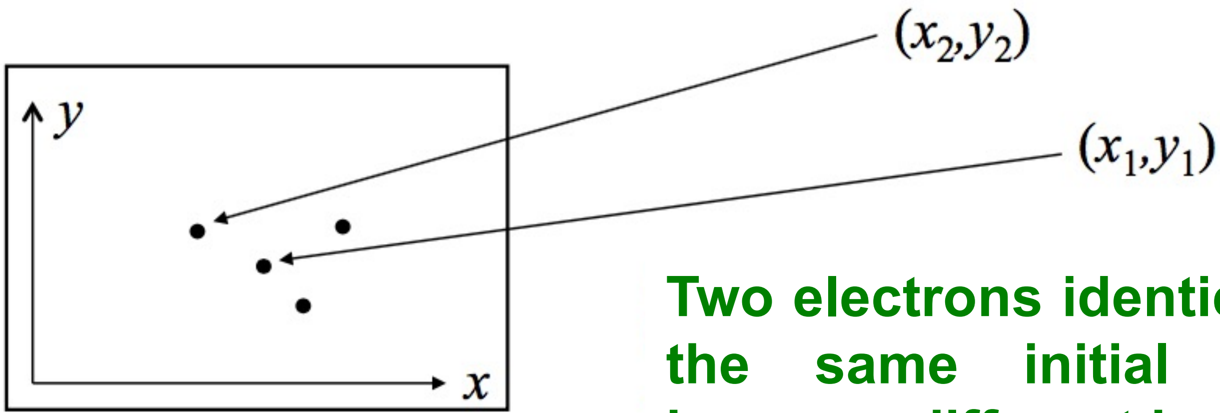
Although electrons are sent one by one, interference fringes could be observed. These interference fringes are formed only when electron waves pass through on both sides of the electron biprism at the same time but nothing other than this

Double slit experiment with electrons



At the beginning, bright spots begin to appear here and there at random positions. Electrons are detected one by one as punctual particles

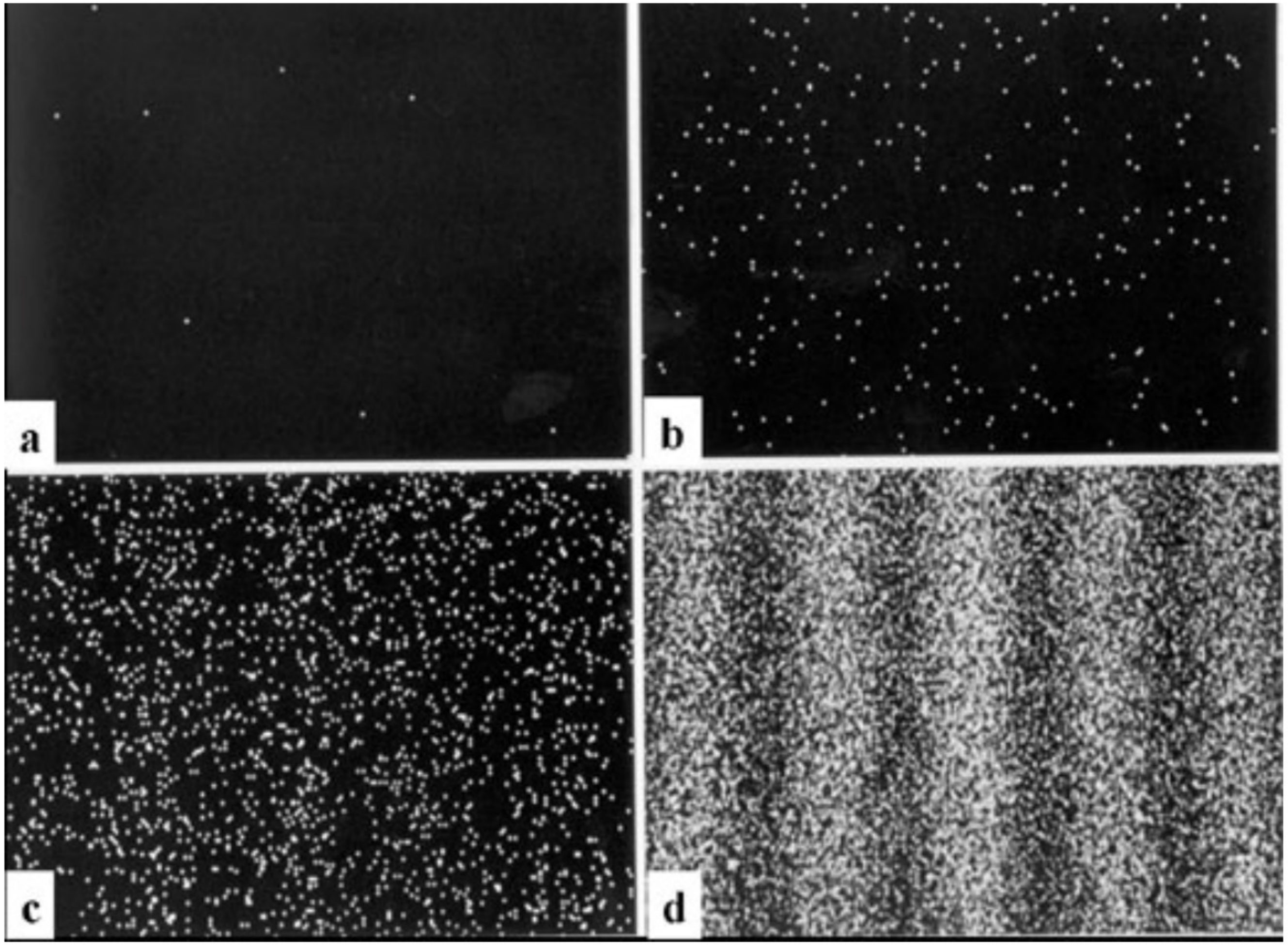
The electron impact point (x,y) looks somewhat random ??



Two electrons identically prepared with the same initial conditions show however different impact points

Double slit experiment with electrons

Double slit experiment with electrons



Number of electrons accumulated: (a) 8; (b) 270; (c) 2,000; (d) 16,000. About 30 minutes is needed to reach stage (d)

The wave function

First postulate: The state of a quantum mechanical system is completely specified by a wavefunction

$\psi(\vec{r}, t)$ **that depends on the spatial coordinates** $\vec{r} = (x, y, z)$

The wavefunction or state function has the important property that is the probability that the particle lies in a volume element located at $\vec{r}$ **and at time t**

$$d^3P = |\psi(\vec{r}, t)|^2 \, d^3r$$

The wavefunction must satisfy certain mathematical conditions because of this probabilistic interpretation

$\psi(\vec{r}, t)$ **probability amplitude**

$|\psi(\vec{r}, t)|^2$ **probabilty density**

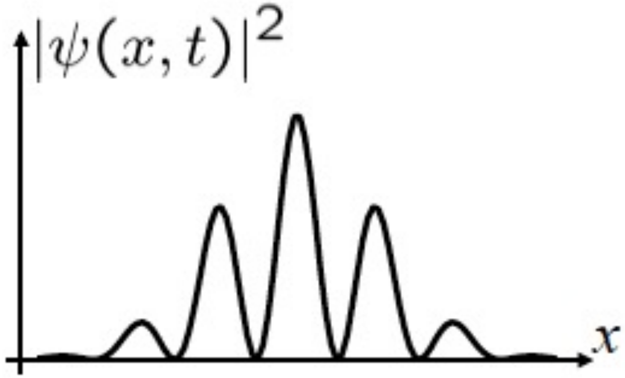
$$\int |\psi(\vec{r}, t)|^2 \, d^3r = 1$$

Normed function

Probabilistic interpretation

Assume N particles identically prepared in the same quantum state

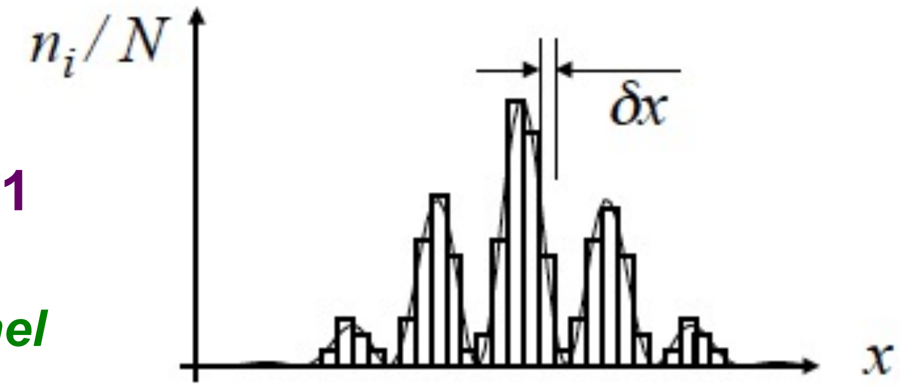
$$\psi(x,t)$$



For each particle, we measure the position with a detector having a spatial resolution δx, then we build-up an histogram of the results

It is possible to retrieve $|\psi(x,t)|^2$ with a good precision if and only if N >> 1

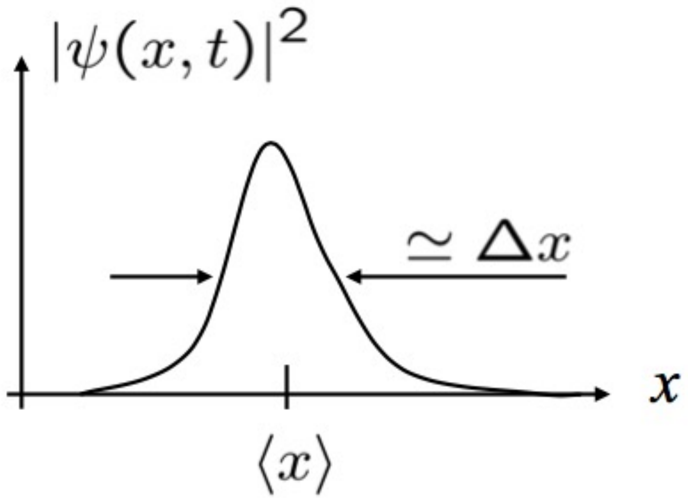
n_i: number of atoms detected in the i^{th} channel



Mean value and root mean square

Mean (expectation) value

$$\langle x \rangle = \int x \underbrace{|\psi(x,t)|^2 \, dx}_{dP(x)}$$



Variance

$$\Delta x^2 = \langle x^2 \rangle - (\langle x \rangle)^2$$

with $$\langle x^2 \rangle = \int x^2 \underbrace{|\psi(x,t)|^2 \, dx}_{dP(x)}$$

Standard deviation or dispersion

$$\Delta x = \sqrt{\Delta x^2}$$

Summary of the 1st postulate

The wave function contains all the information of the system e.g. there is nothing else in the quantum formalism that would allow to know, before doing a measurement where the particle will be detected

The probabilism character and randomness behavior does not result from a lack of knowledge of the initial conditions but is inherently included in the quantum formalism

No hidden variables, "*God does not play dice with the Universe*" (Einstein)

Experiment and theoretical proofs, Bell's theorem

Superposition principle

The wavefunction is a complex-valued probability amplitude

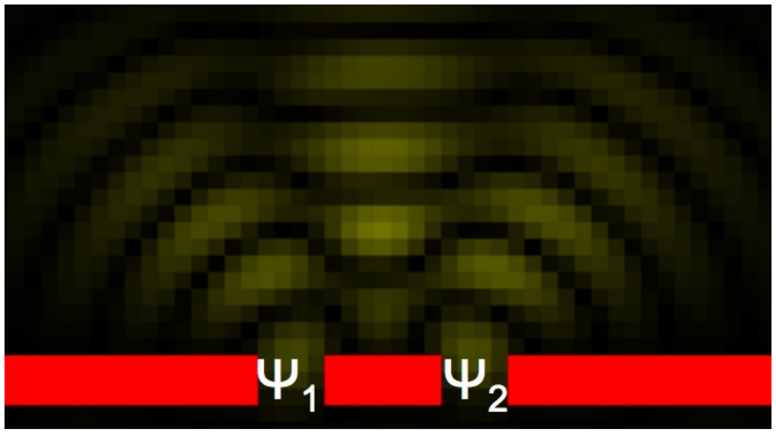
If ψ_1 and ψ_2 are wavefunctions with laws of probability $P_1 = |\psi_1|^2$ and $P_2 = |\psi_2|^2$

then,

$$\psi \propto \psi_1 + \psi_2$$

is also a possible wave function with the law of probability

$$P = |\psi|^2 \propto P_1 + P_2 + \underbrace{\psi_1^* \psi_2 + \psi_1 \psi_2^*}_{\text{Interferences}}$$



Superposition principle is a prerequisite for a structure of a vector space

3.

Schrödinger's equation

(free particle)

 1933

What equation for this wave?

Maxwell equations (vacuum)

$$\vec{\nabla} \cdot \vec{E} = 0, \;\; \vec{\nabla} \cdot \vec{B} = 0$$

$$\frac{\partial}{\partial t}\begin{pmatrix} \vec{E} \\ \vec{B} \end{pmatrix} = \begin{pmatrix} c^2 \, \vec{\nabla} \times \vec{B} \\ -\vec{\nabla} \times \vec{E} \end{pmatrix}$$

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Maxwell equations (vacuum)

$$\vec{\nabla}\cdot\vec{E} = 0,\ \ \vec{\nabla}\cdot\vec{B} = 0$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\vec{E}\\ \vec{B}\end{pmatrix} = \begin{pmatrix} c^2\,\vec{\nabla}\times\vec{B}\\ -\vec{\nabla}\times\vec{E}\end{pmatrix} \quad\Rightarrow\quad \frac{\partial\psi}{\partial t} = F(\psi)$$

$F(\psi)$s a function of ψ and its partial derivatives with respect to the spatial variables (x,y,z)

Solutions: plane waves $\psi = \psi_0\, e^{i(\vec{k}.\vec{r}-\omega t)}$

What equation for this wave?

Let us use the following dispersion relations

The frequency and the wavevector $\omega \longleftrightarrow \vec{k}$

The energy and the momentum $E \longleftrightarrow \vec{p}$

And the link between wave and corpuscle is give by $E = \hbar\omega \quad \vec{p} = \hbar\vec{k}$

	Light	Matter
Corpuscle	$E = cp$ X ħ Einstein	$E = \dfrac{p^2}{2m}$
Wave	$\omega = ck$	/ ħ $\omega = \dfrac{\hbar k^2}{2m}$ de Broglie

What equation for this wave?

Maxwell equations (vacuum)

$$\vec{\nabla} \cdot \vec{E} = 0, \quad \vec{\nabla} \cdot \vec{B} = 0$$

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Hint:

$$\vec{\nabla}\left(e^{i\vec{k}\cdot\vec{r}}\right) = i\vec{k}\, e^{i\vec{k}\cdot\vec{r}}$$

$$\Delta\left(e^{i\vec{k}\cdot\vec{r}}\right) = -k^2\, e^{i\vec{k}\cdot\vec{r}}$$

and $\omega = \dfrac{\hbar k^2}{2m}$

$F(\psi)$?

What equation for this wave?

Maxwell equations (vacuum)

$$\vec{\nabla}\cdot\vec{E}=0,\ \ \vec{\nabla}\cdot\vec{B}=0$$

$$\frac{\partial}{\partial t}\begin{pmatrix}\vec{E}\\ \vec{B}\end{pmatrix}=\begin{pmatrix}c^2\,\vec{\nabla}\times\vec{B}\\ -\vec{\nabla}\times\vec{E}\end{pmatrix}$$

What we want:

$$\frac{\partial\psi}{\partial t}=F(\psi)$$

$F(\psi)$ is a function of ψ and its partial derivatives with respect to the spatial variables (x,y,z)

Solutions: plane waves $\psi=\psi_0\,e^{i(\vec{k}.\vec{r}-\omega t)}$

Finally we get,

$$F(\psi)=i\frac{\hbar}{2m}\Delta\psi$$

Second postulate

The wave function or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi$$

Free particle without interaction

De Broglie's waves are solutions of Schrödinger equation

Quiz n°1

By integrating of the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi$$

What do you get?

1. $\psi(x,t)$ as a function of $\psi(x,0)$
2. $\psi(x,t)$ as a function of $\psi(x,0)$ and $\dfrac{\partial\psi}{\partial t}$ (for t=0)
3. $\psi(x,t)$ as a function of $|\psi(x,0)|^2$

Quiz nº1

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What do you get?

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2. $\psi(x,t)$ as a function of $\psi(x,0)$ and $\frac{\partial\psi}{\partial t}$ (at t=0)
3. $\psi(x,t)$ as a function of $|\psi(x,0)|^2$

See the proof on slide 57

Corollary of the 2nd postulate

Norm conservation

$$\frac{\partial \psi}{\partial t} = i\frac{\hbar}{2m}\Delta\psi \quad \text{and} \quad \frac{\partial \psi^*}{\partial t} = -i\frac{\hbar}{2m}\Delta\psi^*$$

$$\Rightarrow \quad \frac{d}{dt}\int |\psi(\vec{r},t)|^2 \, d^3r = 0$$

Try to demonstrate it !

Paramount of importance because $|\psi|^2$ is a probability density

de Broglie's waves are solutions of the Schrödinger's equation

$$\psi(\vec{r},t) = \psi_0 \, e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)} = \psi_0 \, e^{i(\vec{p}\cdot\vec{r}-Et)/\hbar}$$

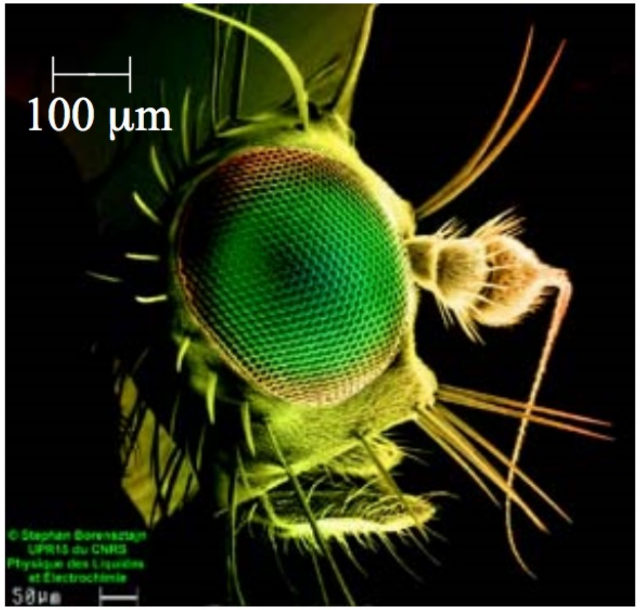
De Broglie's waves are not normalized e.g a plane wave would have to fill all space and thus would require infinite energy!

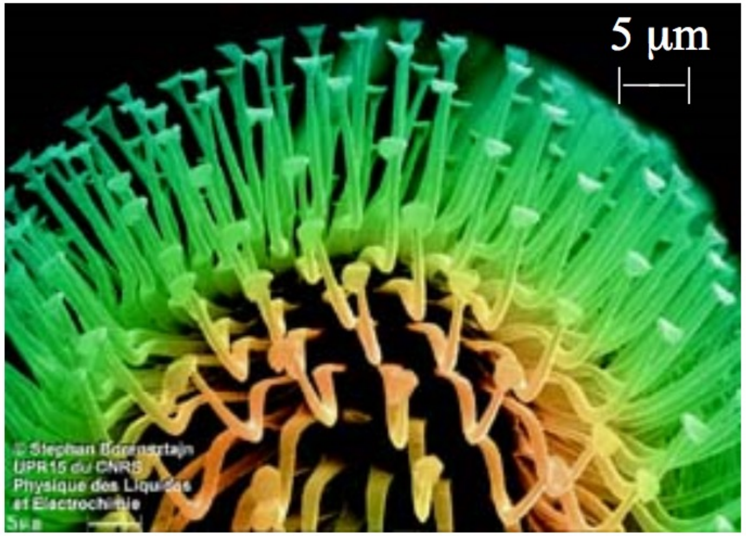
Applications of de Broglie's waves

The resolving power of a microscope is limited by the wavelength, typically a fraction of micrometers with visible light

With an electronic waves operating at much shorter wavelengths, it is possible to access the tiny details of the structure of matter

$$E_{\mathrm{cin}} = 150 \text{ eV} \qquad v = 7\ 10^6 \text{ m/s} \qquad \lambda = 1 \text{ Å}$$

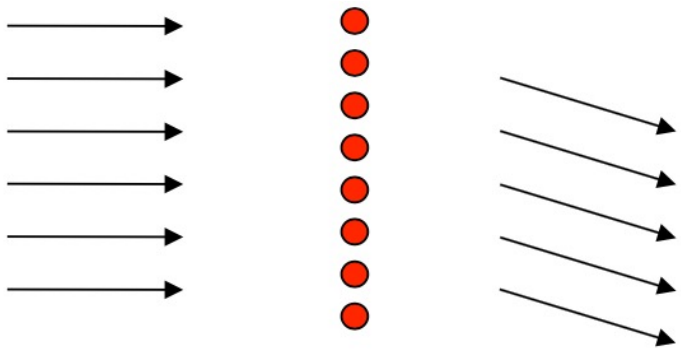




S. Borensztajn, CNRS

Applications of de Broglie’s waves

Coherent Bragg diffraction



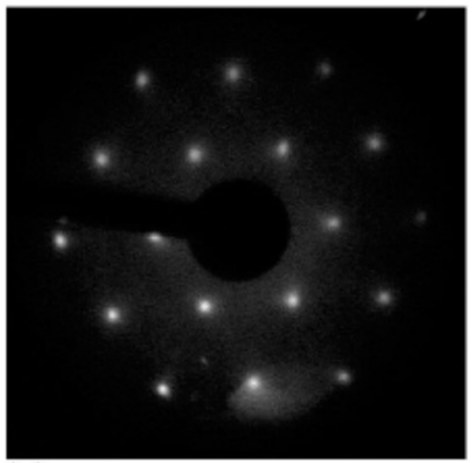
The crystal has a period of a few Angstroms e.g. the wavelength of the probe must be adjusted accordingly

$$\lambda = 1\ \text{Å}$$

electrons $v = 7.3\ 10^6\ \text{m/s}$ $E = 150\ \text{eV}$

neutrons $v = 4000\ \text{m/s}$ $E = 0.1\ \text{eV}$

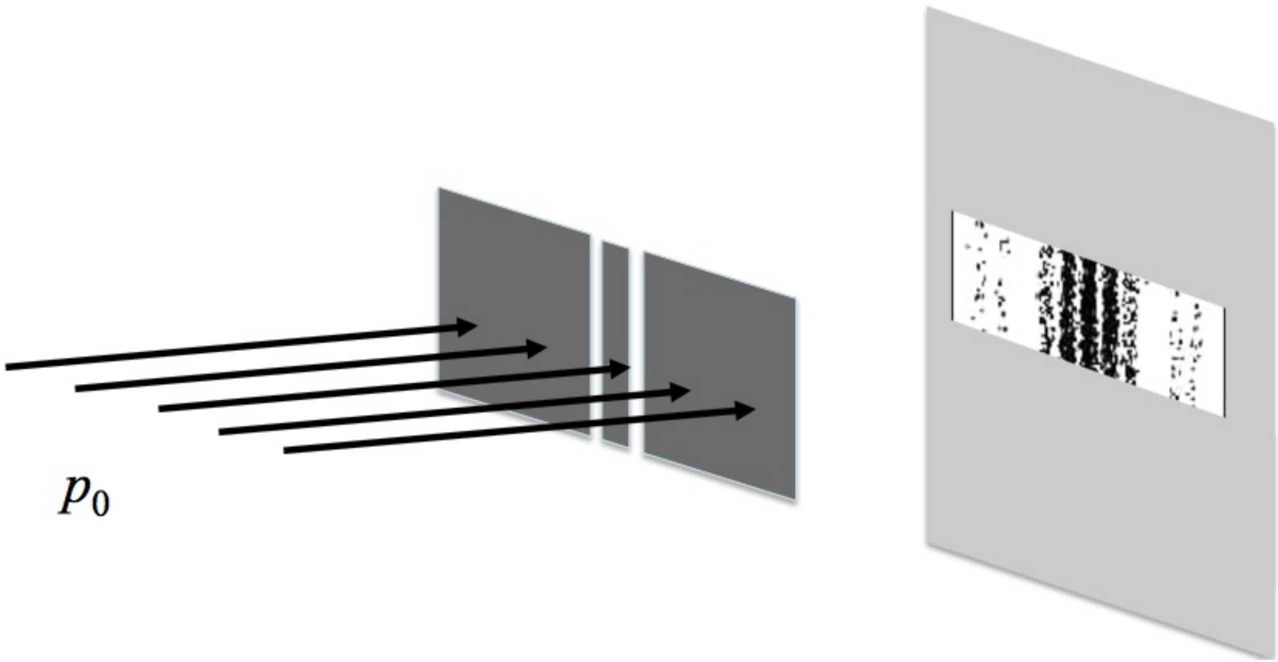
Diffraction pattern of a potassium layer deposited on a crystal graphite



Penn. State University, PRB 70, 245407 (2007)

4.

Which way?



What we know

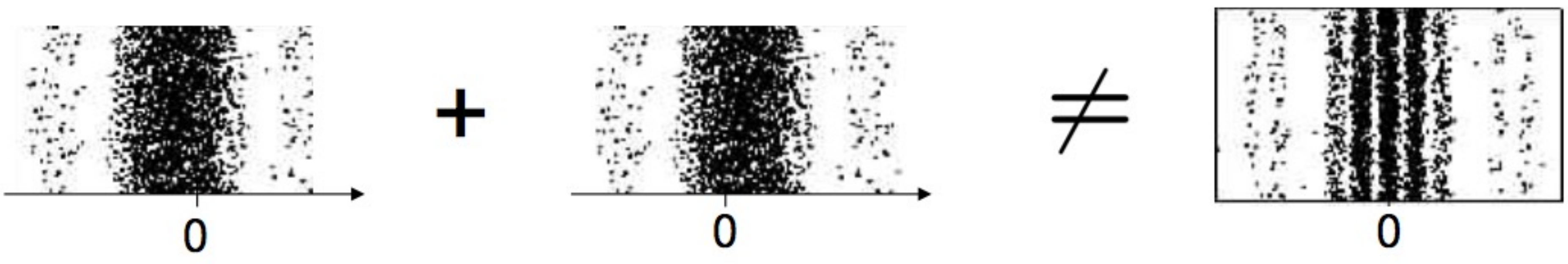
The knowledge of the way followed by the particles (if available) would definitely ruin the fundamental concepts of quantum mechanics.

If slit 1 is left open, we would not observe any interference but only a diffraction pattern. Same conclusion if slit 2 is left open.

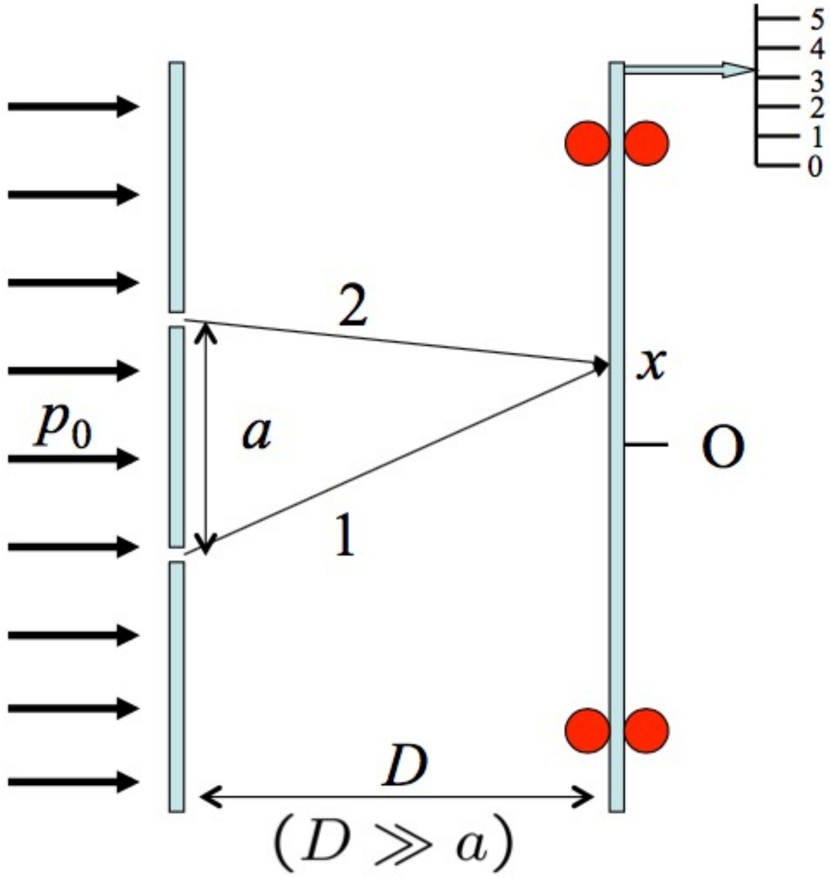
→ The particle passes through slit 1
→ The particle passes through slit 2

$\left.\right\}$ Events

But,



A possible way to track the path



We measure simultaneously the impact point x of the particle and the setback direction of the screen along (Ox)

Path 1 $$p_x^{(1)} = p_0 \frac{x + \frac{a}{2}}{D}$$

Path 2 $$p_x^{(2)} = p_0 \frac{x - \frac{a}{2}}{D}$$

Difference between the two setback momentums

$$p_x^{(1)} - p_x^{(2)} = \frac{a p_0}{D}$$

How to distinguish the paths?

To distinguish the two events, *"the particle passes through slit 1" or "the particle passes through slit 2"*, we have to know the momentum of the screen before each detection with a precision such as

$$\Delta p_x \ll \frac{a p_0}{D}$$

Screen

To observe the interference fringes, we have to position the screen before each detection with a precision such as

$$\Delta x \ll \frac{\lambda D}{a}$$

Fringe interval

$$\lambda = \frac{h}{p_0} \quad \Rightarrow \quad \Delta p_x \, \Delta x \ll h$$

How to distinguish the paths?

We will see later on that it is impossible to prepare a system (particle, screen, etc.) in a state where both the position and the momentum are simultaneously known

$$\Delta x \ \Delta p_x > \frac{\hbar}{2}$$

Using a wheeled screen does not allow to identify the way followed by the particles while observing interference fringes

Quantum mechanics requires to precise the experimental protocol

→ **We can make an experiment where interference are observed**

→ **We can make an experiment where the path followed by the particle is identified**

→ **But we can not do both at the same time**

Relationships for a free particle

	Classical mechanics	Quantum mechanics
Intrinsic characteristics	Mass m Charge q	Mass m Charge q
State of the particle	Position $\vec{r}(t)$ Momentum $\vec{p}(t)$	Wave function $\psi(\vec{r},t)$
Equation of motion	$\frac{d\vec{r}}{dt} = \frac{\vec{p}}{m}$ $\frac{d\vec{p}}{dt} = 0$	$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi$
Type	deterministic $\vec{r},\ \vec{p}$	random $d^3P = \lvert\psi(\vec{r},t)\rvert^2\ d^3r$

Section 2

Position and velocity of a quantum particle

The general Schrödinger's equation

Joseph Fourier
1768-1830

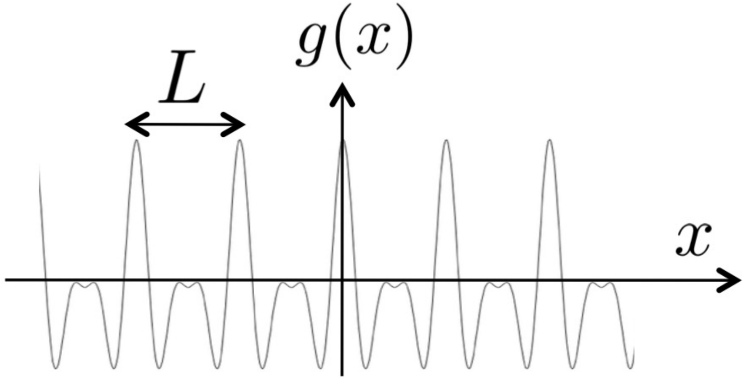
William R. Hamilton
1805-1865

1.

Fourier transform

1768-1830

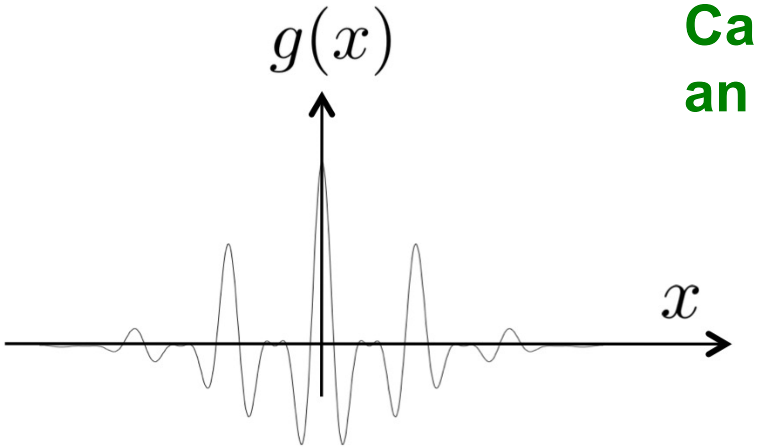
From Fourier series to Fourier transform



Periodic function g(x) of class C^2

$$g(x) = \sum_{n=-\infty}^{+\infty} f_n \, e^{in\xi_0 x} \qquad \xi_0 = \frac{2\pi}{L}$$

with $f_n = \dfrac{1}{L}\displaystyle\int_0^L g(x)\, \mathrm{e}^{-in\xi_0 x} dx$



Can we express an aperiodic function g(x) as an integral over a continuum of exponentials?

$$g(x) \overset{?}{=} \int_{-\infty}^{+\infty} f(\xi)\, \mathrm{e}^{i\xi x} d\xi$$

C∞: smooth functions with rapid decrease (see Schwartz's space)

Definition

In Mathematics, the FT is defined in L[1] space (integrable functions)

$$f \longrightarrow \hat{f} \qquad\qquad \hat{f}(\xi) := \int_{\mathbf{R}^N} \mathrm{e}^{-\mathrm{i}\xi\cdot x}\, f(x)\, \mathrm{d}x$$

In Physics, the TF is defined in L[2] space (square-integrable functions)

$$\psi \longrightarrow \varphi \qquad\qquad \varphi(p) := \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}xp/\hbar}\, \psi(x)\, \mathrm{d}x$$

$xp/\hbar$ = dimensionless x = position $\hbar$ = J/s p = momentum

The Schwartz's space S is used in quantum mechanics. It represents rapidly decreasing functions C^∞ e.g. a function f(x) such that f(x), f′(x), f″(x), ... all exist everywhere and go to zero as x → ±∞ faster than any inverse power of x

Properties

If $\psi(x)$ is known, we can calculate $\varphi(p)$ by using

$$\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ixp/\hbar}\, \psi(x)\, dx$$

Is it also possible to retrieve $\psi(x)$ when the FT $\varphi(p)$ is known?

YES! $$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ixp/\hbar}\, \varphi(p)\, dp$$

By definition: $\varphi(p)$ is the direct FT of $\psi(x)$

$\psi(x)$ is the inverse FT of $\varphi(p)$

$$e^{\pm ixp/\hbar}$$

Position $\psi(x) \xleftrightarrow{\text{FT}} \varphi(p)$ Momentum

Properties

Isometry of the Fourier transform

$$\psi_1(x) \overset{\textbf{FT}}{\longleftrightarrow} \varphi_1(p) \qquad \psi_2(x) \overset{\textbf{FT}}{\longleftrightarrow} \varphi_2(p)$$

Isometry $$\int \psi_1^*(x)\,\psi_2(x)\,\mathrm{d}x = \int \varphi_1^*(p)\,\varphi_2(p)\,\mathrm{d}p$$

Compact notation $\langle \psi_1 | \psi_2 \rangle = \langle \varphi_1 | \varphi_2 \rangle$ ***Scalar product (see Hilbert's space)***

Normalization conditions

$$1 = \int |\psi(x)|^2\,\mathrm{d}x = \int |\varphi(p)|^2\,\mathrm{d}p$$

Compact notation $1 = \langle \psi | \psi \rangle = \langle \varphi | \varphi \rangle$ ***Scalar product***

Properties

Derivatives and Fourier transform? $\psi(x) \xleftrightarrow{\text{FT}} \varphi(p)$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ixp/\hbar}\, \varphi(p)\, dp$$

There is no issue in taking the derivatives under the integral term which is okay owing to the Schwartz's space

$$\frac{\mathrm{d}\psi(x)}{\mathrm{d}x} = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ixp/\hbar} \left[\frac{ip}{\hbar}\varphi(p)\right] \mathrm{d}p \qquad \frac{\mathrm{d}\psi(x)}{\mathrm{d}x} \xleftrightarrow{\text{FT}} \frac{ip}{\hbar}\varphi(p)$$

$$\frac{d^2\psi(x)}{dx^2} = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ixp/\hbar} \left[-\frac{p^2}{\hbar^2}\varphi(p)\right] dp \qquad \frac{d^2\psi(x)}{dx^2} \xleftrightarrow{\text{FT}} -\frac{p^2}{\hbar^2}\varphi(p)$$

Taking the derivatives in the position space = multiplication by $ip/\hbar$ **in the momentum space**

Schrödinger's equation (free particle)

Let consider the initial condition (t=0) of the wavefunction be: $\psi(x,0)$

We search the solution $\psi(x,t)$ of the Schrödinger's equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

Let us use the Fourier transform

$$\psi(x,t) \longleftrightarrow \varphi(p,t) \quad \Rightarrow \quad \frac{\partial^2\psi(x,t)}{\partial x^2} \longleftrightarrow -\frac{p^2}{\hbar^2}\varphi(p,t)$$

The FT of the Schrödinger's equation is $\quad i\hbar\frac{\partial\varphi(p,t)}{\partial t} = \frac{p^2}{2m}\varphi(p,t)$

This equation easily be integrated $\quad \varphi(p,t) = \varphi(p,0)\, e^{-ip^2t/(2m\hbar)}$

with $\quad |\varphi(p,t)|^2 = |\varphi(p,0)|^2$

Schrödinger's equation (free particle)

The evolution of the Fourier transform for any t is given by:

$$\varphi(p,t) = \varphi(p,0)\, e^{-ip^2 t/(2m\hbar)}$$

To retrieve $\psi(x,t)$ we use the inverse Fourier transform

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \varphi(p,t)\, e^{ipx/\hbar}\, dp$$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \varphi(p,0)\, \mathrm{e}^{-ip^2 t/(2m\hbar)}\, \mathrm{e}^{ixp/\hbar}\, dp$$

Initial conditions $\varphi(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x,0)\, \mathrm{e}^{-ixp/\hbar}\, dx$

→ general method to solve the Schrödinger's equation (free-particle)

Momentum of the free particle

If the particle is in a quantum state $\psi(x)$, the associated probability distribution for the momentum is such as

$$\mathcal{P}(p) = |\varphi(p)|^2 \qquad \psi(x) \xleftrightarrow{\text{FT}} \varphi(p)$$

We know that if $\psi(x)$ is normed then $\int \mathcal{P}(p)\, dp = 1$

And we have seen that $|\varphi(p,t)|^2 = |\varphi(p,0)|^2$

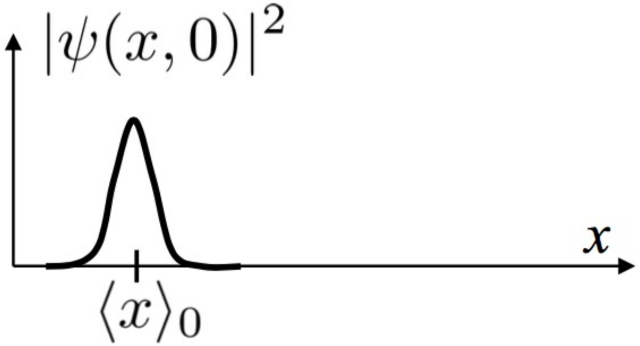
e.g. the quantity $\mathcal{P}(p)$ is not time-dependent (free particle)

In classical mechanics, once the trajectory of the particle x(t) is known, we can calculate the momentum. Does that remain true in quantum mechanics?

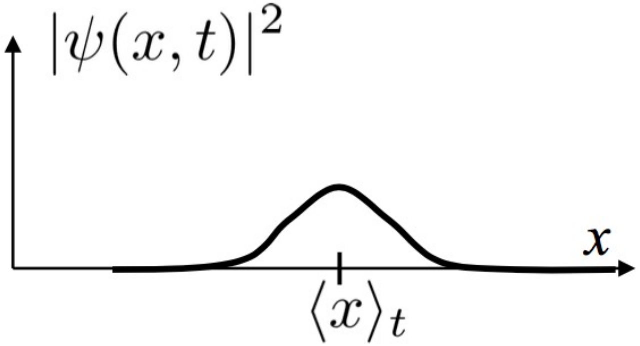
$$p = m\frac{\mathrm{d}x}{\mathrm{d}t} \quad \Rightarrow \quad \langle p\rangle_t = m\frac{\mathrm{d}\langle x\rangle_t}{\mathrm{d}t} \quad ?$$

Momentum of the free particle

Time evolution of the mean position (Gaussian wavepacket)



$$\langle x \rangle_0 = \int x \, |\psi(x,0)|^2 \, \mathrm{d}x$$



$$\langle x \rangle_t = \int x \, |\psi(x,t)|^2 \, \mathrm{d}x$$

Do we find $\langle p \rangle_t = m \dfrac{\mathrm{d}\langle x \rangle_t}{\mathrm{d}t}$ **when** $\langle p \rangle_t$

is defined as $\langle p \rangle_t = \int p \, |\varphi(p,t)|^2 \, \mathrm{d}p$ **?**

Momentum of the free particle

Let us try to re-express $\langle p \rangle = \int p \, |\varphi(p)|^2 \, \mathrm{d}p$ **as a function of** $\psi(x)$

First, we write the mean momentum as follows $\langle p \rangle = \int \varphi^*(p) \, p \, \varphi(p) \, \mathrm{d}p$

Isometry $$\int \varphi_1^*(p) \, \varphi_2(p) \, \mathrm{d}p = \int \psi_1^*(x) \, \psi_2(x) \, \mathrm{d}x$$

$$\varphi_1(p) = \varphi(p) \quad \xleftrightarrow{\textbf{FT}} \quad \psi_1(x) = \psi(x)$$

Derivative $$\varphi_2(p) = p \, \varphi(p) \quad \xleftrightarrow{\textbf{FT}} \quad \psi_2(x) = \frac{\hbar}{i} \frac{\mathrm{d}\psi(x)}{\mathrm{d}x}$$

$$\boxed{\langle p \rangle = \int \psi^*(x) \, \frac{\hbar}{i} \frac{\mathrm{d}\psi(x)}{\mathrm{d}x} \, \mathrm{d}x}$$

Momentum of the free particle

The evolution of the mean position of the particle is given by

$$\frac{\mathrm{d}\langle x\rangle_t}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\int x\,\psi^*(x,t)\,\psi(x,t)\,\mathrm{d}x \quad = \int x\,\psi^*\,\frac{\partial\psi}{\partial t}\,\mathrm{d}x + \int x\,\frac{\partial\psi^*}{\partial t}\,\psi\,\mathrm{d}x$$

Then we have to use the Schrödinger's equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \qquad\qquad -i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}$$

Integration by parts assuming

ψ → **0 for** $|x| \rightarrow \infty$

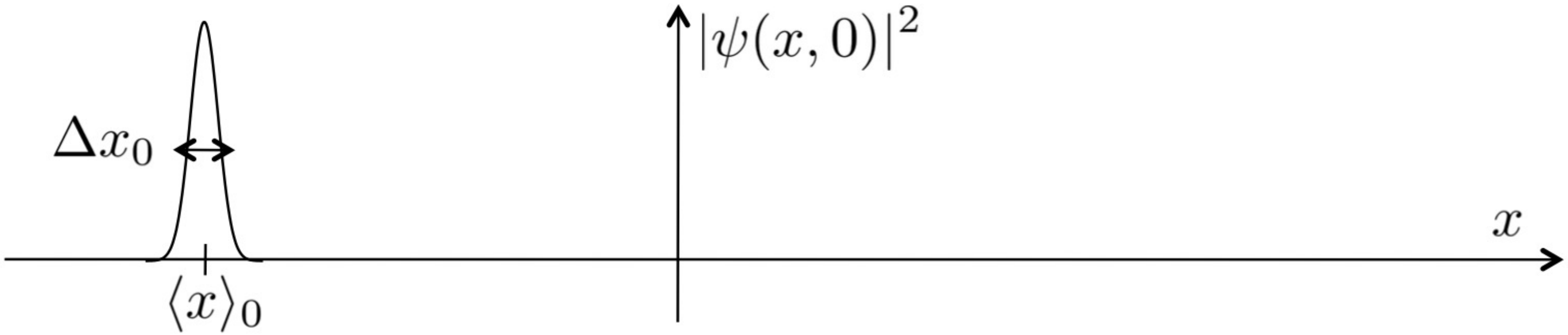
Try to demonstrate it (not trivial)

$$\frac{d\langle x\rangle_t}{dt} = \int \psi^*\,\frac{\hbar}{im}\,\frac{\partial\psi}{\partial x}$$

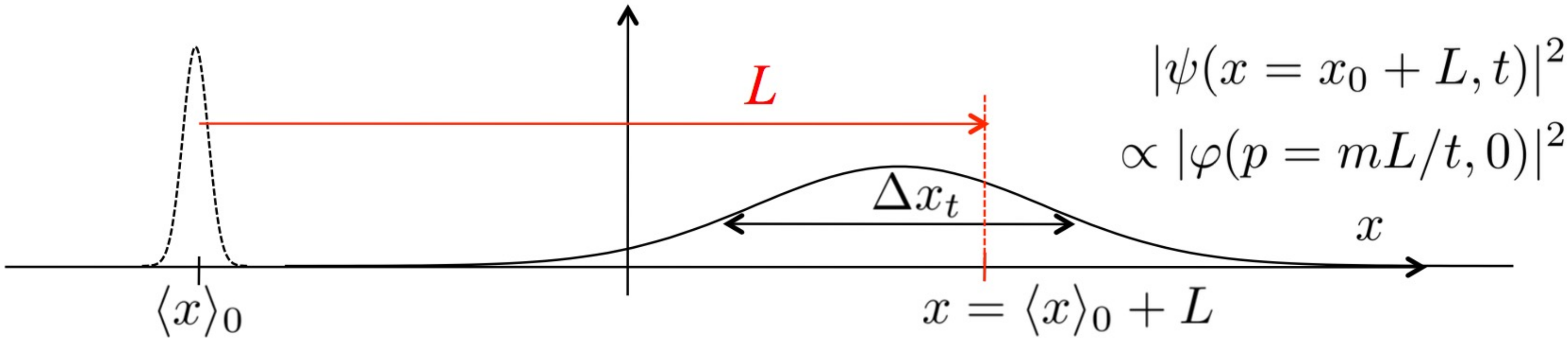
$$m\frac{d\langle x\rangle_t}{dt} = \int \psi^*\,\frac{\hbar}{i}\,\frac{\partial\psi}{\partial x} = \langle p\rangle_t$$ **QED**

Momentum of the free particle

At t=0, the wavefunction of the particle is $\psi(x,0)$



Time of flight measurement: after a certain time such as $\Delta x_t >> \Delta x_0$ it is possible to show that the position distribution reproduces precisely the momentum distribution $|\varphi(p,0)|^2$



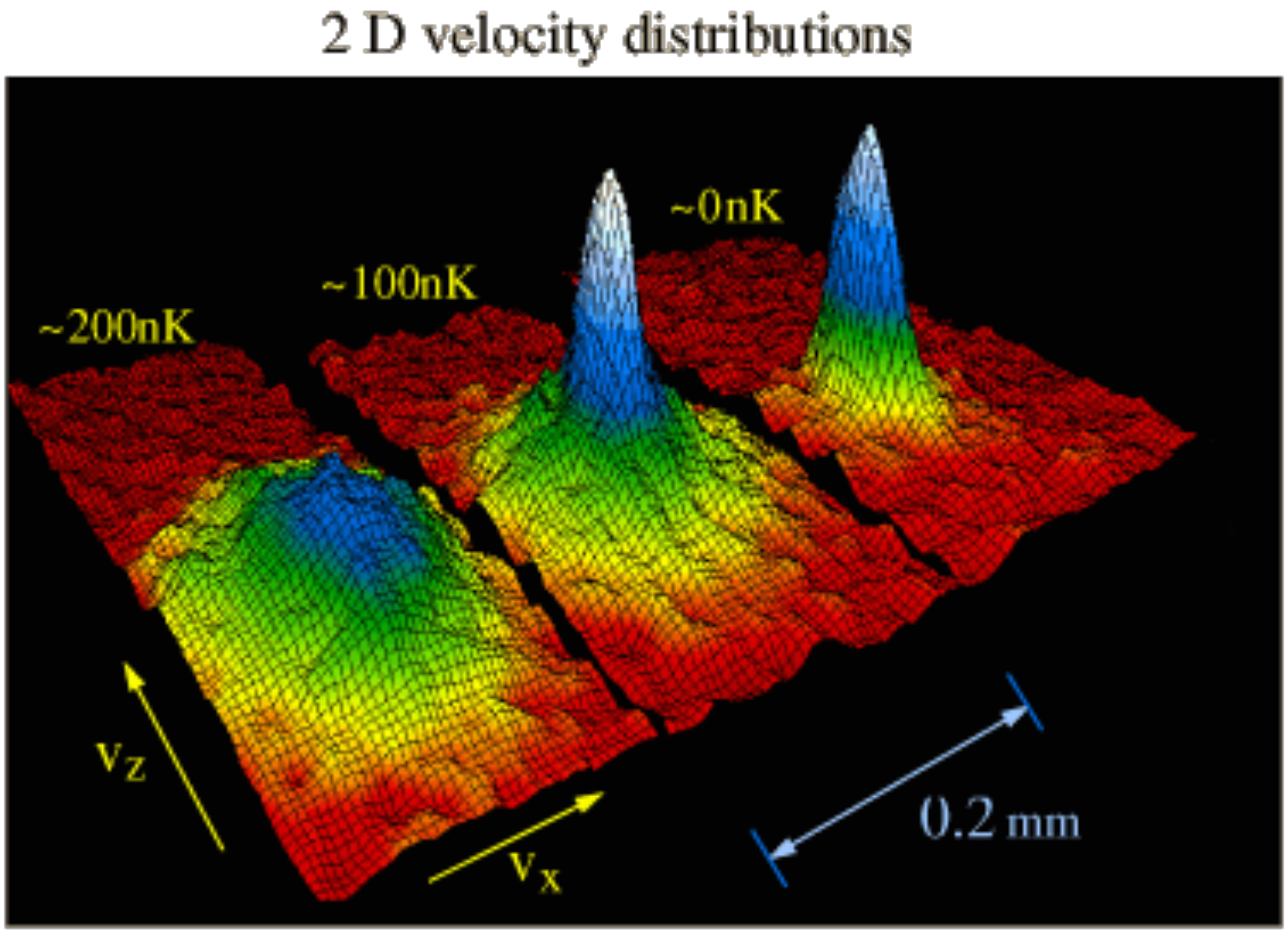
Measurement used in cold atom experiments to determine the momentum distribution of atoms in the optical trap

Bose-Einstein condensates

Bosons can condense in unlimited numbers into a single ground state and not constrained by the Pauli exclusion principle

Bose-Einstein condensates

Bosons can condense in unlimited numbers into a single ground state and not constrained by the Pauli exclusion principle



JILA, University of Colorado, United States

2.

Position, momentum, energy operators

General Schrödinger's equation

Position and momentum

Mean position $$\langle x\rangle = \int x\,|\psi(x)|^2\,\mathrm{d}x = \int \psi^*(x)\,x\,\psi(x)\,\mathrm{d}x$$

Mean momentum $$\langle p\rangle = \int p\,|\varphi(p)|^2\,\mathrm{d}p = \int \psi^*(x)\,\frac{\hbar}{i}\frac{\mathrm{d}\psi}{\mathrm{d}x}\,\mathrm{d}x$$

We introduce the position and momentum operators

$$\langle x\rangle = \int \psi^*(x)\,\left[\hat{x}\,\psi(x)\right]\,\mathrm{d}x \qquad \psi(x) \xrightarrow{\hat{x}} x\,\psi(x)$$

$$\langle p\rangle = \int \psi^*(x)\,\left[\hat{p}\,\psi(x)\right]\,\mathrm{d}x \qquad \psi(x) \xrightarrow{\hat{p}} \frac{\hbar}{i}\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}$$

Later on, we will able to generalize the concept of operators to any physical quantities (quantum mechanical observables)

General Schrödinger's equation

We have seen that the evolution of the wavefunction $\psi(x,t)$ for a free particle is driven by the one dimensional equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

We can rewrite this equation using the momentum operator

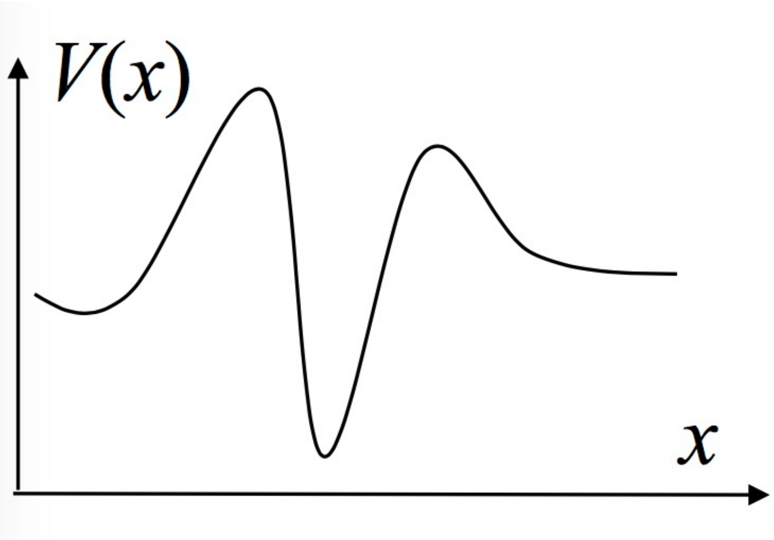
$$i\hbar\frac{\partial\psi}{\partial t} = \frac{\hat{p}^2}{2m}\psi \quad \text{with} \quad \psi(x) \xrightarrow{\hat{p}} \frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}$$

or

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \quad \text{with} \quad \hat{H} = \frac{\hat{p}^2}{2m}$$

$\hat{H}$ is the "kinetic energy operator" which coincides here with the total energy (free particle). The Schrödinger's equation links time and energy

Schrödinger's equation with a potential



The idea is to keep the same structure

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

And we include both kinetic and potential energies to form the Hamiltonian (e.g. total energy operator)

2nd postulate (general case): for a particle of mass m and moving into a potential V(x), the Schrödinger's equation is written such as

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \qquad \textbf{with} \qquad \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

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

Quantum equivalent of the Newton's law of motion in classical physics

3.

Wavepacket

Heisenberg's uncertainty principle

Physical meaning of the Fourier transform

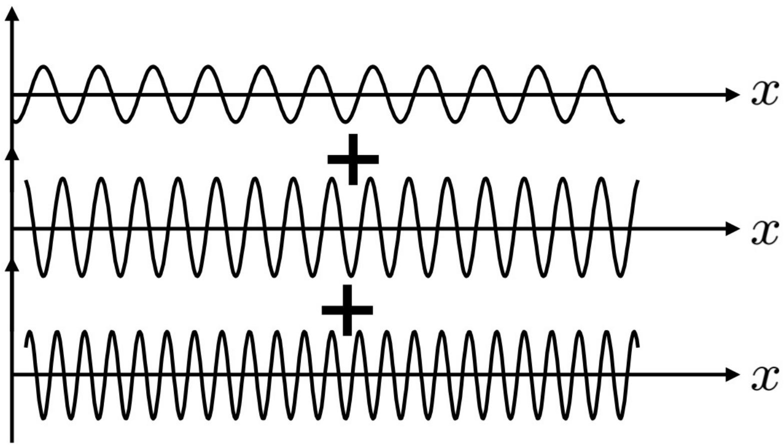
We have seen the existence of de Broglie's wave $\psi(x) = \mathrm{e}^{\mathrm{i}xp_0/\hbar}$

associated to a particle with momentum p_0, ….. but these waves are not normalizable!

We can create a new object e.g. a wavepacket which is a superposition of de Broglie's waves $\mathrm{e}^{\mathrm{i}xp/\hbar}$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{e}^{\mathrm{i}xp/\hbar} \, \varphi(p) \, \mathrm{d}p$$

Amplitude



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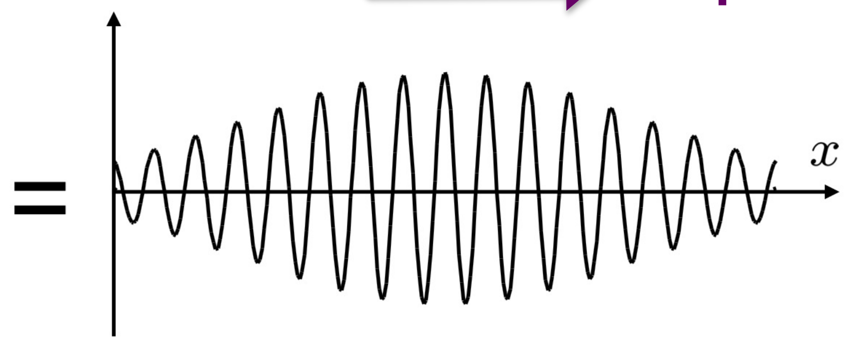


Wavepacket

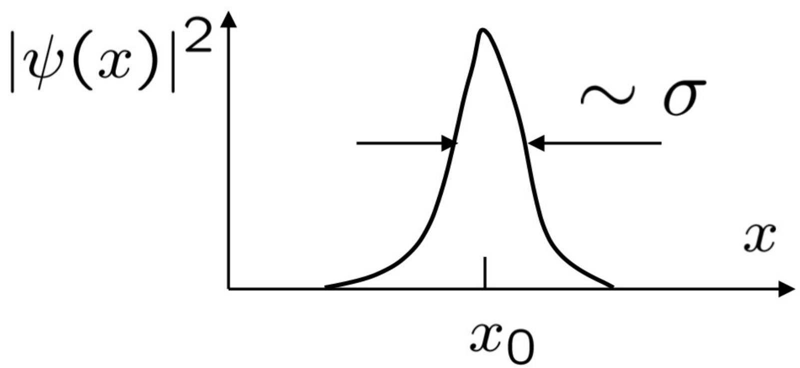
Wavepackets

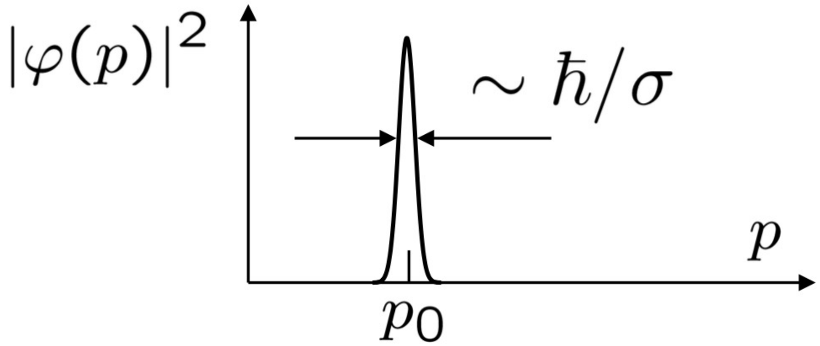
In classical mechanics we can say:
"Let's assume a particle with position x_0 and momentum p_0"

In quantum mechanics we must say:
"Let's assume a particle described by the quantum state $\psi(x)$ and its Fourier transform $\varphi(p)$"

→ With a position probability distribution $|\psi(x)|^2$ centered at x_0

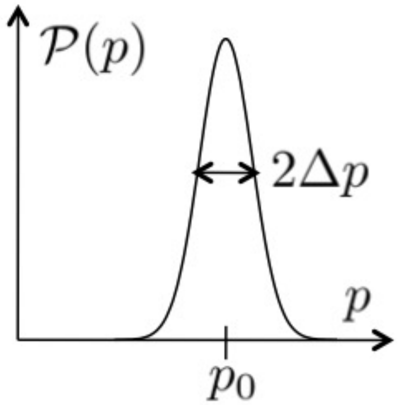
→ With a momentum probability distribution $|\varphi(p)|^2$ centered at p_0





Gaussian wavepacket

Derivations are analytical with Gaussian functions!

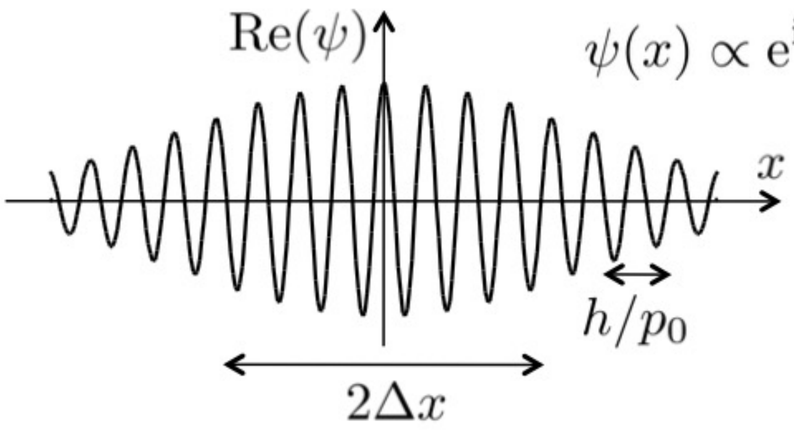


$$\varphi(p) \propto \mathrm{e}^{-(p-p_0)^2/(4q^2)} \qquad \mathcal{P}(p) \propto \mathrm{e}^{-(p-p_0)^2/(2q^2)}$$

Mean $\langle p \rangle = p_0$

Dispersion $\Delta p = q$

What is the corresponding wavefunction $\psi(x)$?



$$\psi(x) \propto \mathrm{e}^{\mathrm{i}p_0 x/\hbar}\,\mathrm{e}^{-q^2x^2/\hbar^2} \qquad \mathcal{P}(x) \propto \mathrm{e}^{-2q^2x^2/\hbar^2}$$

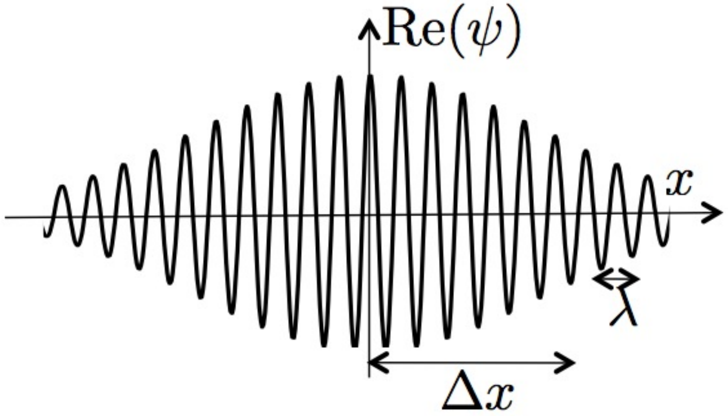
Mean $\langle x \rangle = 0$

Dispersion $\Delta x = \dfrac{\hbar}{2q}$

For a Gaussian wavepacket, we always have $\Delta x\,\Delta p = \dfrac{\hbar}{2}$

Gaussian wavepacket

Quasi monokinetic wavepacket $\Delta p \ll p_0$



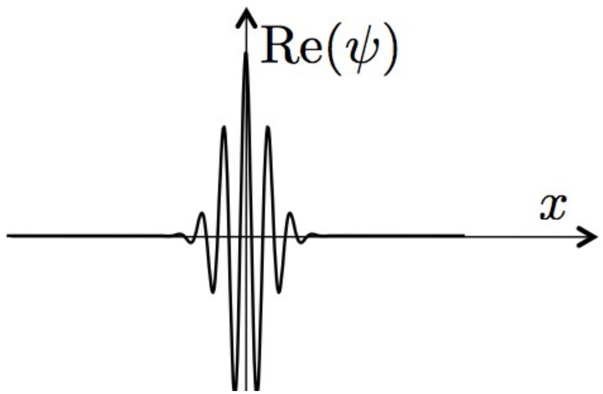
Lots of oscillations are observed

$$\lambda = \frac{h}{p_0} \quad \ll \quad \Delta x = \frac{\hbar}{2\,\Delta p}$$

A plane wave is retrieved!

Well localized wavepacket $\Delta x \approx \lambda$

The momentum is not well defined $\Delta p \approx p_0$



$$\Delta x\, \Delta p = \frac{\hbar}{2}$$

A wavepacket cannot be simultaneously well localized and quasi-monokinetic!

Heisenberg's uncertainty principle

Can we generalize? YES

Position probability distribution for the particle: $\mathcal{P}(x) = |\psi(x)|^2$

$$\Delta x = \left[\langle x^2\rangle - \langle x\rangle^2\right]^{1/2} \qquad \langle x^n\rangle = \int x^n\, |\psi(x)|^2\, dx$$

Momentum probability distribution for the particle: $\mathcal{P}(p) = |\varphi(p)|^2$

$$\Delta p = \left[\langle p^2\rangle - \langle p\rangle^2\right]^{1/2} \qquad \langle p^n\rangle = \int p^n\, |\varphi(p)|^2\, dp$$

We always have : $\boxed{\Delta x\, \Delta p \geq \frac{\hbar}{2}}$

Also true in 3 dimensions : $\Delta x\, \Delta p_x \geq \frac{\hbar}{2},\ \ \Delta y\, \Delta p_y \geq \frac{\hbar}{2},\ \ \Delta z\, \Delta p_z \geq \frac{\hbar}{2}$

Quiz nº2

What does the Heisenberg's uncertainty principle mean?

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

1. It is not possible to prepare a particle in a quantum state such that both the position and momentum are simultaneously well defined

2. The wavepacket spreads out (true but not related to the question)

3. The product of the precisions of the measured position and momentum is larger than the modified Planck's constant

Quiz n°2

What does the Heisenberg's uncertainty principle mean?

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

1. It is not possible to prepare a particle in a quantum state such that both the position and momentum are simultaneously well defined

2. The wavepacket spreads out (true but not related to the question)

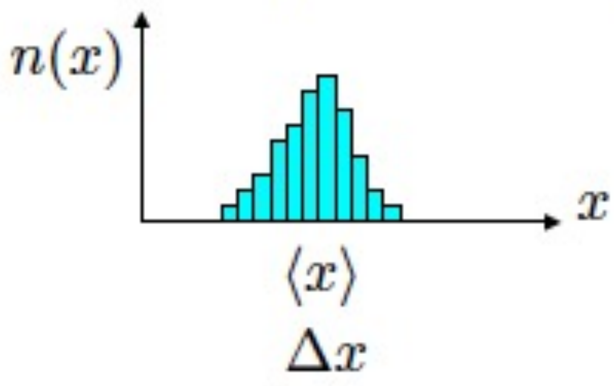
3. The product of the precisions of the measured position and momentum is larger than the modified Planck's constant

Quiz n°2: solution

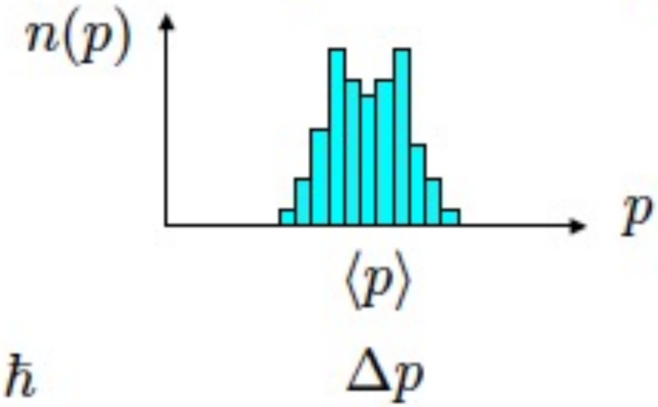
It is not possible to prepare a particle in a state such that both the position and the impulsion are simultaneously well defined

Let us consider 2N particles identically prepared $\psi(x) \xleftrightarrow{\text{FT}} \varphi(p)$

Measured position (N particles)



Measured momentum (N particles)

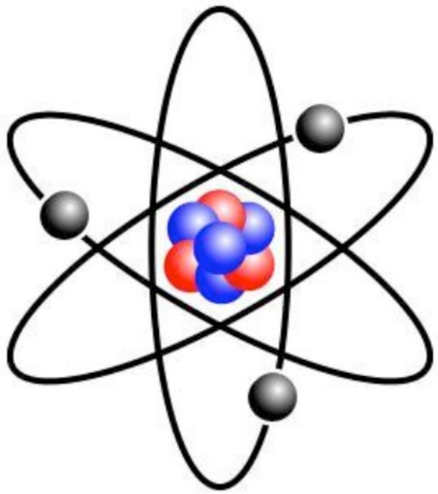


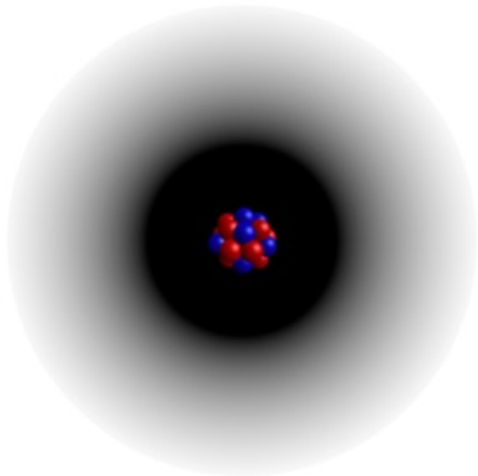
$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

These histograms can not be simultaneously arbitrary narrow. Note that the uncertainty principle has nothing to do with the resolution of the equipment i.e. the width of the histogram's channels

8.

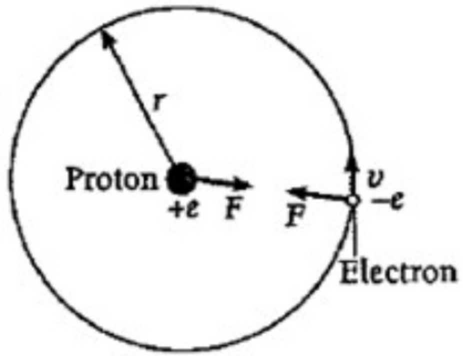
Stability of Quantum Matter





Instability of “classical matter”

The planetary model of the atom does not make sense when one considers the electromagnetic forces involved. The electron in an orbit is accelerating continuously and would thus radiate away its energy and fall into the nucleus



Coulomb potential $V(r) = -e^2/r$ $\quad e^2 = \dfrac{q^2}{4\pi\varepsilon_0}$

Newton’s law $m\omega^2 r = e^2/r^2 \longrightarrow v = \omega r = e/\sqrt{mr}$

Kinetic energy $E_{kin} = \dfrac{1}{2}mv^2 = \dfrac{1}{2}m\dfrac{e^2}{mr} \longrightarrow E_{kin} = \dfrac{e^2}{2r}$

Total energy $E_{tot} = E_{kin} + V(r) = -\dfrac{e^2}{2r}$ $\quad E_{tot} \to -\infty$, $r \to 0$

The classical matter is unstable !

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Instability of "classical matter"

Larmor's formula can be used to calculate the total power radiated by a non relativistic point charge as it accelerates or decelerates

$$\mathcal{P} \sim \frac{e^2 a^2}{c^3} \rightarrow \delta E = 2\pi \frac{\mathcal{P}}{\omega} = 2\pi \frac{e^2 r^2 \omega^3}{c^3}$$

$a = \omega^2 r$ **Acceleration**

c **celerity of light**

Relative energy lost after 1 cycle

$$\omega r = e/\sqrt{mr}$$

$$\frac{\delta E}{|E_{tot}|} \sim 4\pi \left(\frac{\omega r}{c}\right)^3 = 4\pi \left(\frac{e^2/r}{mc^2}\right)^{3/2}$$

Typical values $r = 1\,\text{Å}$ $\omega \approx 2\,10^{16}\,\mathrm{s}^{-1}$

Binding energy

$$\frac{e^2/r}{mc^2} \approx 3\;10^{-5}$$

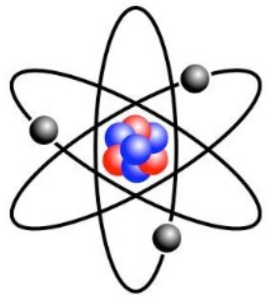
Rest energy

The relative energy lost after one cycle remains small however the electron has an angular rate of rotation of 2 × 10^{16} cycles/s.

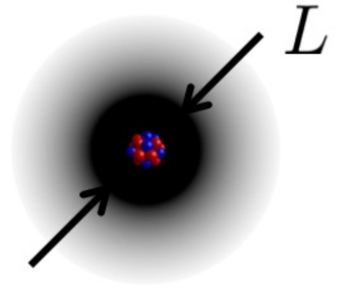
$$m^2 c^3 r^3 / e^4 \approx 0.4\ \text{ns}$$

The electron would fall into the nucleus within 0.4 ns!

Stability of “quantum matter”



Classical physics



Quantum physics

$$\langle \vec{r} \rangle = \langle \vec{p} \rangle = 0$$

$$\Delta x \Delta p_x \geq \hbar/2$$

$$\Delta y \Delta p_y \geq \hbar/2$$

$$\Delta z \Delta p_z \geq \hbar/2$$

$$\Delta x \leq L \quad \longrightarrow \quad \Delta p_x \geq \frac{\hbar}{2L}$$

The uncertainty principle contains implications about the energy that would be required to contain a particle within a given volume

$$E_{kin} = \frac{|\vec{p}|^2}{2m} = \frac{\Delta p^2}{2m} \geq \frac{3\hbar^2}{8mL^2}$$

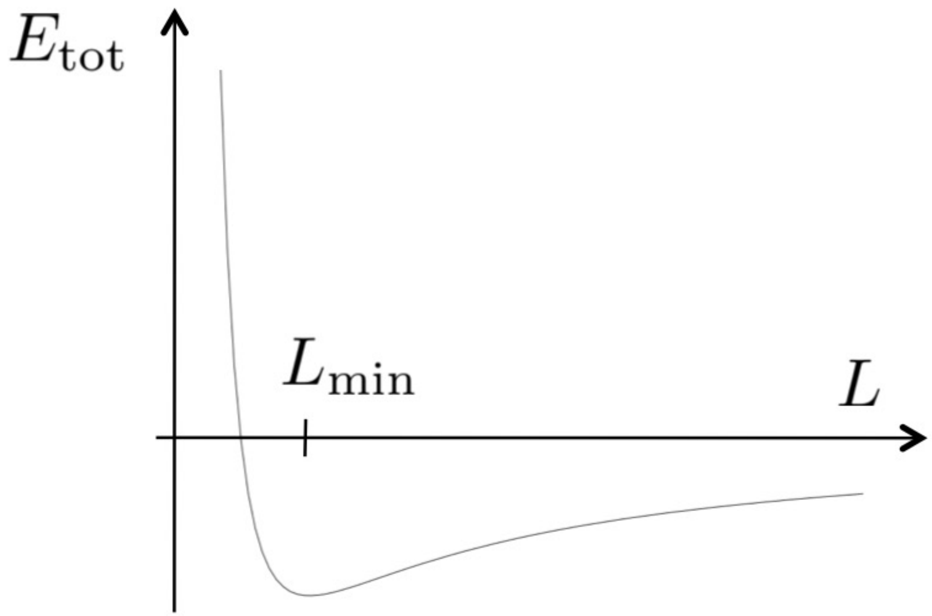
When the radius of the orbit L→0, we observe that the positive kinetic energy overwhelms the negative Coulomb potential!

Stability of "quantum matter"

$$E_{\text{tot}} = E_{kin} + E_{\text{pot}}$$

$$E_{kin} \sim \frac{3\hbar^2}{8mL^2}$$

$$E_{\text{pot}} \sim V(L) = -\frac{e^2}{L}$$



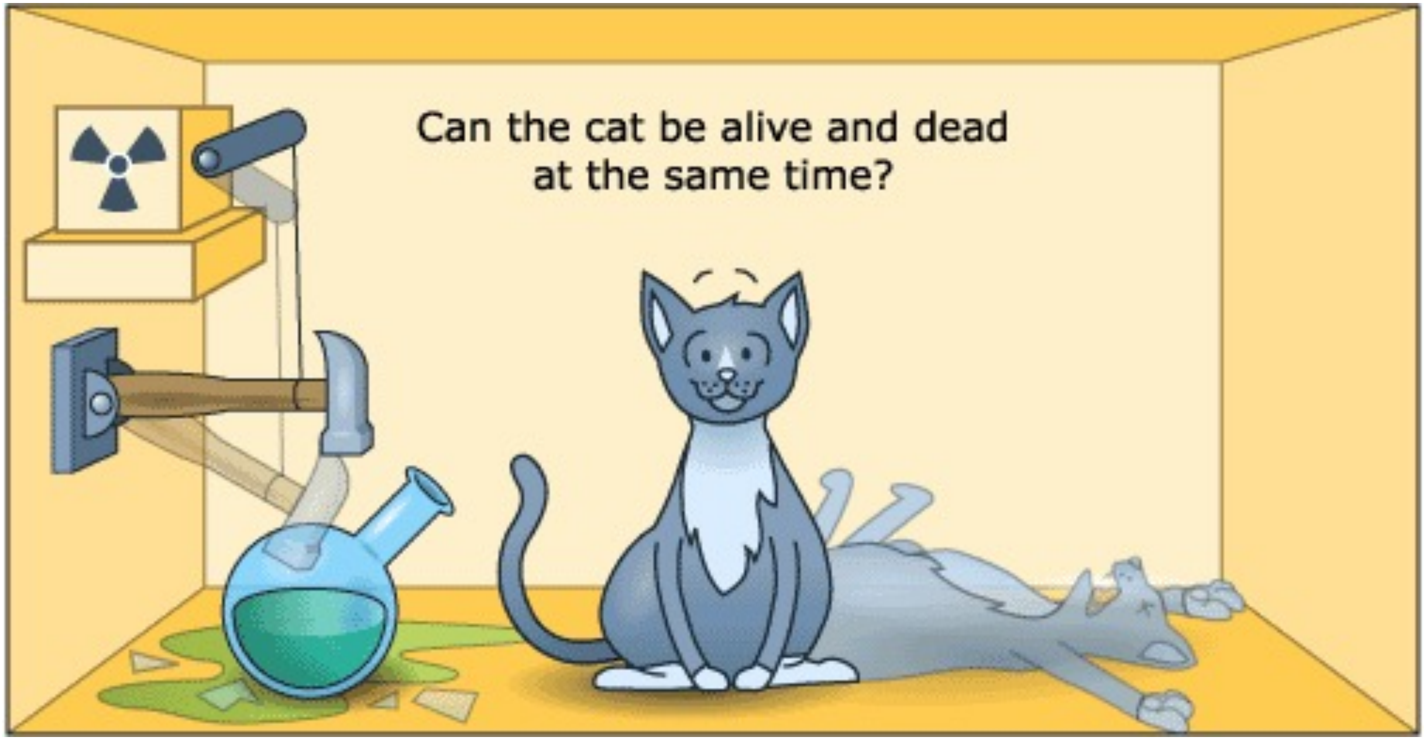
Minimum $\frac{3\hbar^2}{8mL^2} - \frac{e^2}{L}$ **for** $L_{\text{min}} = \frac{3\hbar^2}{4me^2}$

Here we extract the the Bohr's radius of the electron that is the minimum energy state (ignoring a multiplication factor of ¾)

Quantum mechanics tells us that an ATOM COULD NEVER COLLAPSE as it would take an infinite energy to locate the electron on top of the proton

Section 3

Measurements in quantum mechanics



1.

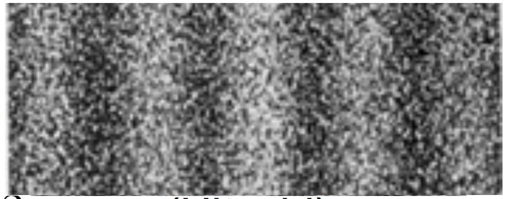
The measurement of physical quantities: position, momentum, & energy

Position and momentum

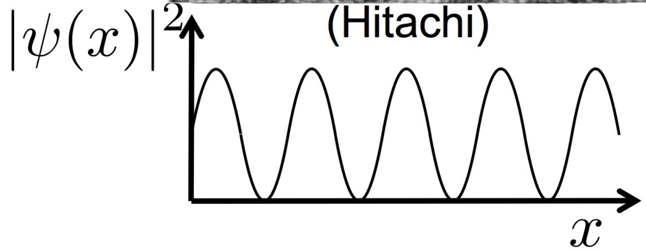
Point particle with wave function $\psi(x)$

Position probability distribution $|\psi(x)|^2$

Expectation $\langle x \rangle = \int x\,|\psi(x)|^2\,dx$



(Hitachi)



Measure of the momentum through a time of flight experiment

$$\psi(x) \overset{\textbf{FT}}{\longleftrightarrow} \varphi(p)$$

$$dP = |\varphi(p)|^2\,dp \qquad (p \equiv p_x)$$

$$\langle p \rangle = \int p\,|\varphi(p)|^2\,dp$$

that is equivalent to $\langle p \rangle = \int \psi^*(x)\,\frac{\hbar}{i}\,\frac{d\psi}{dx}\,dx$

Quiz n°3

Operators and quantum states

1. The operator $\hat{x}$ only acts on the function $\psi(x)$

   and the operator $\hat{p}$ only acts on the function $\varphi(p)$

2. The operators $\hat{x}$ and $\hat{p}$ act both on $\psi(x)$ and $\varphi(p)$

3. The Hamiltonian is the sole operator acting both on $\psi(x)$ and $\varphi(p)$

Quiz n°3

Operators and quantum states

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Operators

Expectation values

$$\langle x \rangle = \int x \, |\psi(x)|^2 \, \mathrm{d}x = \int \psi^*(x) \, x \, \psi(x) \, \mathrm{d}x$$

$$\langle p \rangle = \int p \, |\varphi(p)|^2 \, \mathrm{d}p = \int \psi^*(x) \, \frac{\hbar}{i} \frac{\mathrm{d}\psi}{\mathrm{d}x} \, \mathrm{d}x$$

Inner (scalar) product in L^2 space

$$\langle \psi_1 \mid \psi_2 \rangle = \int \psi_1^*(x) \, \psi_2(x) \, \mathrm{d}x$$

Operators

Position operator

$$\langle x \rangle = \int \psi^*(x)\, [\hat{x}\, \psi(x)]\, dx$$

$$= \langle \psi \mid \hat{x}\psi \rangle$$

$$\psi(x) \xrightarrow{\hat{x}} x\, \psi(x)$$

Momentum operator

$$\langle p \rangle = \int \psi^*(x)\, [\hat{p}\, \psi(x)]\, dx$$

$$= \langle \psi \mid \hat{p}\psi \rangle$$

$$\psi(x) \xrightarrow{\hat{p}} \frac{\hbar}{i} \frac{d\psi(x)}{dx}$$

$$\hat{p} \equiv \hat{p}_x$$

3^{rd} postulate (weak version)

To every observable in classical mechanics A there corresponds a linear, Hermitian operator $\hat{A}$ in quantum mechanics

$\hat{A}$ is an operator acting on the wave function space

If a system is in a state described by a normalized wave function $\psi(x)$ then, the average value $\langle a \rangle$ of the observable corresponding to $\hat{A}$ is

$$\langle a \rangle = \int \psi^*(x) \left[\hat{A}\psi(x)\right] \mathrm{d}x = \langle \psi \mid \hat{A}\psi \rangle$$

Hermitian operator

$$\int \psi_1^*(x) \left[\hat{A}\psi_2(x)\right] dx = \int \left[\hat{A}\psi_1(x)\right]^* \psi_2(x) dx \quad \Rightarrow \quad \langle a \rangle \in \mathbb{R}$$

$$\langle \psi_1 \mid \hat{A}\psi_2 \rangle = \langle \hat{A}\psi_1 \mid \psi_2 \rangle$$

Physical quantity	Action of the corresponding op. on $\psi(\vec{r})$
Position $x\,,\; y\,,\; z\,,\; \vec{r}$	Multiplication by $x\,,\; y\,,\; z\,,\; \vec{r}$
Momentum $p_x\,,\; p_y\,,\; p_z$ $\vec{p},\; p^2$	$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$ $\quad \hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$ $\quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$ $\hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}$ $\quad \hat{p^2} = -\hbar^2\Delta$
Total energy $E = \frac{p^2}{2m} + V(\vec{r})$	Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{\vec{r}})$ $= -\frac{\hbar^2}{2m}\Delta + V(\vec{r})$
Angular momentum $\vec{L} = \vec{r}\times\vec{p}$ $L_z = xp_y - yp_x$	Angular momentum operator $\hat{\vec{L}} = \hat{\vec{r}}\times\hat{\vec{p}}$ $\hat{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$

2.

Eigenvalues and eigenfunctions of operators in quantum mechanics

Definition

An eigenfunction of an operator $\hat{A}$ defined on the wave function space is any non-zero function $\psi_\alpha(x)$ in that space that, when acted upon by $\hat{A}$ is only multiplied by some scaling factor called an

eigenvalue a_α

$$\hat{A}\psi_\alpha(x) = a_\alpha\,\psi_\alpha(x)$$

Spectral theorem: If the operator $\hat{A}$ is Hermitian, there exist an orthonormal basis of consisting of eigenvectors of $\hat{A}$

→ Each eigenvalue is element of the set of real numbers $\mathbb{R}$

→ The operator $\hat{A}$ is diagonalizable

Note the occurrence of some subtleties when moving to a complex space with an infinite-dimension! (see later on)

Example: The momentum operator

Let us search the eigenvalues and eigenfunctions of the momentum operator

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$$

$$\hat{p}\psi_q(x) = q\,\psi_q(x)$$

with q Eigenvalue

$\psi_q(x)$ Eigenfunctions

$$\frac{d\psi_q}{dx} = \frac{iq}{\hbar}\psi_q \quad \Rightarrow \quad \psi_q(x) = C\,e^{iqx/\hbar}$$

→ The eigenfunctions of the momentum operator are the plane waves

→ The spectral distribution of the momentum (e.g. the set of eigenvalues) is the whole set of real numbers $\mathbb{R}$

Eigenfunctions of the Hamiltonian

Play a crucial role to describe the evolution of many quantum systems

$$\hat{H}\psi_E(x) = E\,\psi_E(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + V(x)\,\psi_E(x) = E\,\psi_E(x)$$

1 D

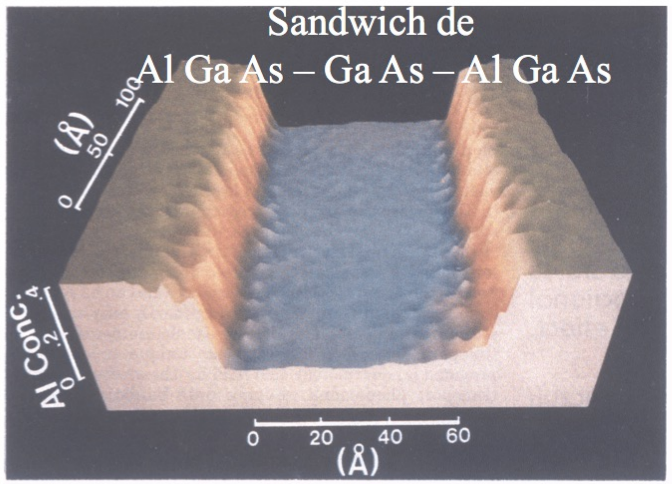
Solutions usually not trivial (→ numerical analysis)

Some cases can be solved analytically

Harmonic potential $V(x) = \frac{1}{2}m\omega^2 x^2$

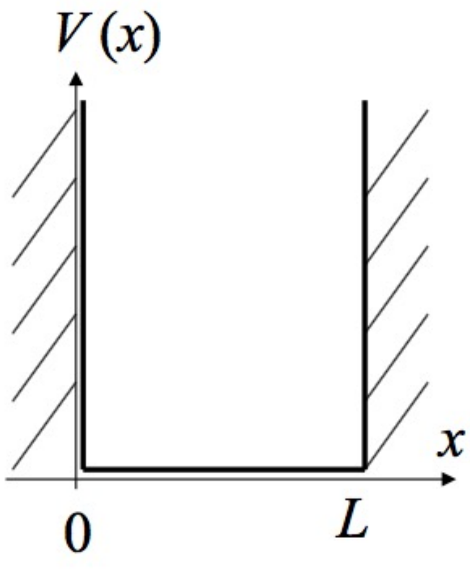
Coulomb potential $V(r) = -\frac{q^2}{4\pi\epsilon_0 r}$

Constant piecewise potentials



Infinite well potential

Particle in a box



$$\hat{H}\psi_E(x) = E\,\psi_E(x)$$

To simplify we assume $\psi_E(x) \equiv \psi(x)$

x	$0 \leq x \leq L$	$x < 0$ ou $x > L$
	$-\dfrac{\hbar^2}{2m}\psi''(x) = E\,\psi(x)$	$\psi(x) = 0$

Boundary conditions: The wave function is always continuous!

$$\psi(0) = \psi(L) = 0$$

Infinite well potential

We assume the energy E >0 and $\in \mathbb{R}$ $k = \sqrt{2mE}/\hbar$ $\qquad E = \hbar^2 k^2/2m$

$$-\frac{\hbar^2}{2m}\psi''(x) = E\,\psi(x) \quad \Rightarrow \quad \psi''(x) = -k^2\,\psi(x)$$

General form of the solutions $\psi(x) = \alpha\sin(kx) + \beta\cos(kx)$

Boundary at $x = 0$ **:** $\psi(0) = 0 \;\Rightarrow\; \beta = 0$

Boundary at $x = L$ **:** $\psi(L) = 0 \;\Rightarrow\; \alpha\sin(kL) = 0 \;\Rightarrow\; \sin(kL) = 0$

→ All wavevectors k can take only discrete values

$$k = k_n = \frac{n\pi}{L} \qquad n = 1, 2, \ldots$$

→ And all eigenvalues of the energy are quantized $E_n = n^2\dfrac{\hbar^2\pi^2}{2mL^2}$

Infinite well potential

Eigenfunctions of the Hamiltonian can be expressed as follows

$$\psi_n(x) = \alpha \sin(k_n x) \quad \textbf{with} \quad k_n = \frac{n\pi}{L} \quad \textbf{and} \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Normalization $\displaystyle\int_0^L |\psi_n(x)|^2 \, dx = 1 \quad \Rightarrow \quad \alpha = \sqrt{2/L}$

The set of functions ψ_n is an orthonormal base of functions such as

$$\psi(0) = \psi(L) = 0$$

Orthonormality $\displaystyle\int_0^L \psi_n(x) \, \psi_\ell(x) \, dx = \delta_{n,\ell}$ ***(Kronecker delta)***

The wave function can be represented by the expansion

$$\psi(x) = \sum_{n=1}^{+\infty} C_n \, \psi_n(x) \qquad \sum_{n=1}^{+\infty} |C_n|^2 = 1$$

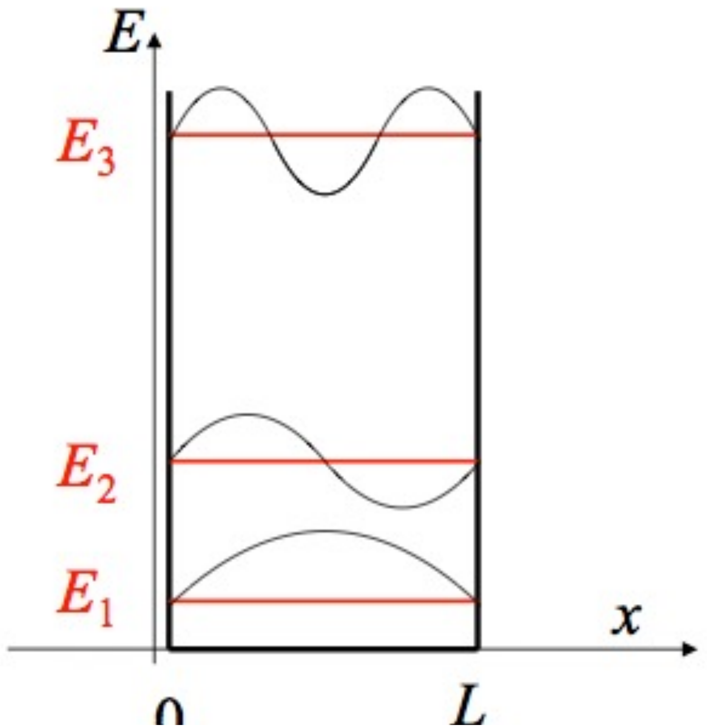
Similar to a Fourier series expansion
Similar to a decomposition in a vector subspace

Infinite well potential

$$E_n = n^2 E_1 \qquad n = 1, 2, \ldots$$

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2}$$

$$\psi_n(x) \propto \sin(n\pi x / L)$$



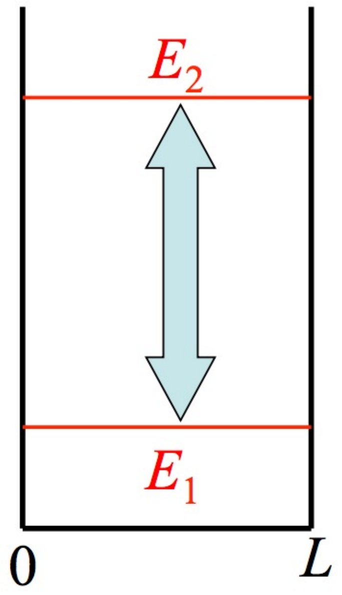
→ **An electron in a quantum well of diameter L = 6 × 10^{-9} m**

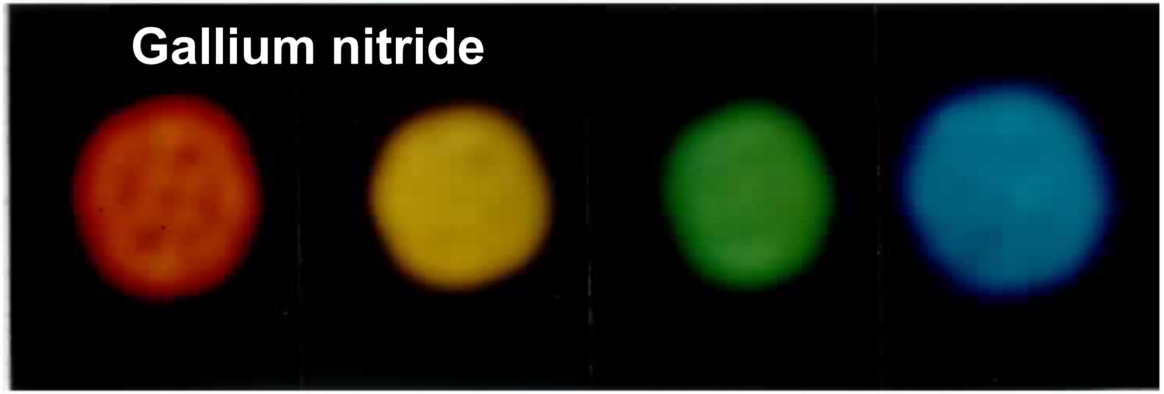
E_1=10 meV

→ **A nucleon (proton or neutron) in a nucleus of diameter L = 4 × 10^{-15} m**

E_1=10 MeV

Light emission from a quantum well





$L = 12$ L **Atomic layers** $L = 6$

Photon $h\nu = E_2 - E_1 = hc/\lambda$

$$E_2 - E_1 = (4-1) \times \frac{\hbar^2 \pi^2}{2mL^2}$$
$$= \frac{3\hbar^2\pi^2}{2mL^2}$$

The Nobel Prize in Physics 2014

Isamu Akasaki, Hiroshi Amano, Shuji Nakamura

"for the invention of efficient blue light-emitting diodes which has enabled bright and energy-saving white light sources"

A key application: Semiconductor lasers

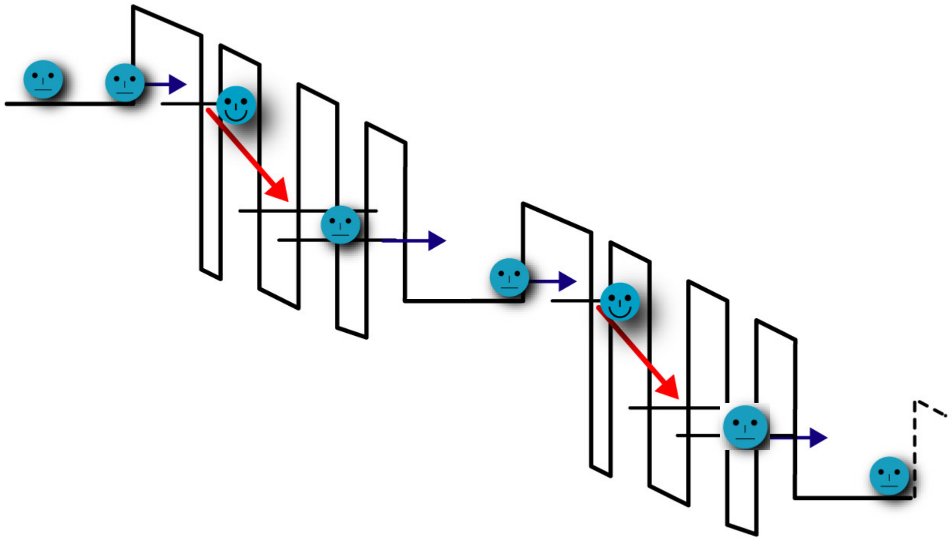
Optical communications

Gas/molecule detection

→ Medical (breath analyses)

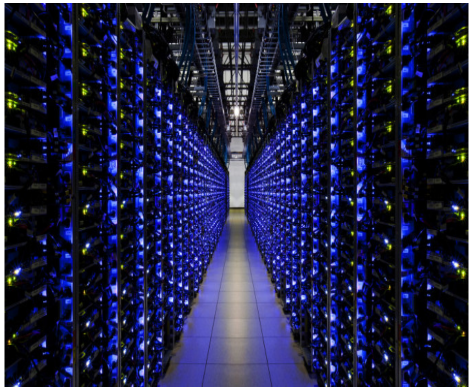
→ Environment (air pollution)

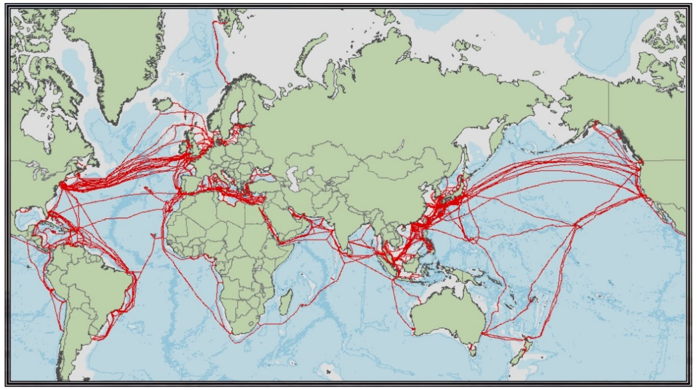
→ Security (explosive detectio



Countermeasures

Atmospheric communications





Diode lasers and quantum cascade lasers can produce stimulated light from near infrared to THz range!

3.

What results for a single measurement?

Relationship between measured results and eigenvalues?

We want to measure a physical quantity A of a particle prepared in the quantum state $\psi(x)$

The result of the measurement of A is predicted with certainty if and only if the state $\psi(x)$ is an eigenstate of observable $\hat{A}$

Proof:

If $\psi(x) = \psi_\alpha(x)$ the measure of A is predicted with certainty

$$\langle a \rangle = \int \psi_\alpha^*(x)\,[\hat{A}\psi_\alpha(x)]\,dx = \int \psi_\alpha^*(x)\,[a_\alpha \psi_\alpha(x)]\,dx = a_\alpha$$

QED

$$\langle a^2 \rangle = \int \psi_\alpha^*(x)\,[\hat{A}^2\psi_\alpha(x)]\,dx = a_\alpha^2 \qquad \Rightarrow \quad \Delta a^2 = \langle a^2 \rangle - (\langle a \rangle)^2 = 0$$

Example: we found that an eigenstate of the Hamiltonian corresponds to an energy level of the quantum well (particle in a box)

Relationship between measured results and eigenvalues?

Converse?

$$\langle a \rangle = \int \psi^*(x)\,[\hat{A}\psi(x)]\,dx \qquad\qquad \Delta a^2 = 0$$

We assume the system in the state $\psi(x)$ in such way that the physical quantity A is well defined (no fluctuations among the measured results)

Then, $\psi(x)$ is an eigenstate of $\hat{A}$ with the corresponding eigenvalue $\langle a \rangle$

Proof

$$0 = \int \psi^*(x)\,[(\hat{A} - \langle a \rangle)^2 \psi(x)]\,dx$$

$$= \int [(\hat{A} - \langle a \rangle)\psi(x)]^* \,[(\hat{A} - \langle a \rangle)\psi(x)]\,dx$$

$$(\hat{A} - \langle a \rangle)\psi(x) = 0 \qquad \Rightarrow \quad \hat{A}\psi(x) = \langle a \rangle\,\psi(x)$$

QED

Relationship between measured results and eigenvalues?

Converse?

$$\langle a \rangle = \int \psi^*(x)\,[\hat{A}\psi(x)]\,dx \qquad\qquad \Delta a^2 = 0$$

We assume the system in the state $\psi(x)$ in such way that the physical quantity A is well defined (no fluctuations among the measured results)

Then, $\psi(x)$ is an eigenstate of $\hat{A}$ with the corresponding eigenvalue $\langle a \rangle$

Conclusion: The measurement of A is predicted with certainty if and only if the state of the particle is an eigenstate of $\hat{A}$

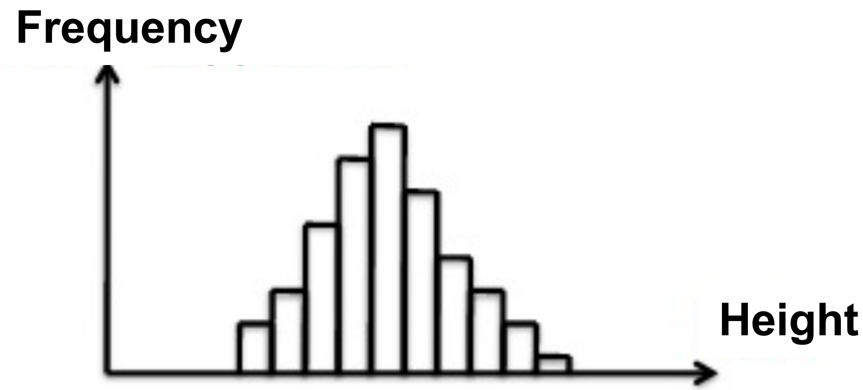
→ The result is the associated eigenvalue (must be a real number)

→ An eigenstate is basically a state without dispersion

What to expect from a measurement?

The measurement of a physical quantity gives a number (or a set of numbers) which brings information on the system under study

Ex: Distribution of human height

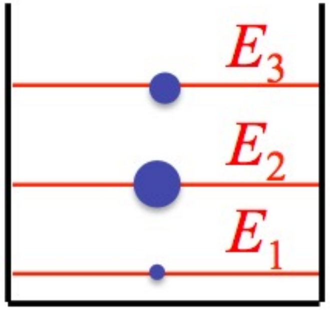


The result is trustable if and only if the measurement of a physical quantity done over a short period of time gives the same numbers (repeatability)

A short period of time means that the state of the system does not substantially evolve between two consecutive measurements (i.e. same experimental conditions)

Which state after the measurement?

Energy levels in a quantum well



Initial state

$$\psi(x) = \sum_n C_n \psi_n(x)$$

Time t_1

Measurement of energy

Result is ε

What are the possible values?

State after the measurement?

Time t_2

Another measurement on the same system at t_2 and performed immediately after t_1 must give the same result with certainty

The measurement performed at t_2 is predicted with certainty if and only if:

(a) The energy ε must be an eigenvalue of the energy operator i.e. is an element of the set of the eigenvalues E_n

(b) The system has to be in an eigenstate of the energy operator at t_2

Measurement at t_1: $\psi(x) \longrightarrow \psi_n(x)$

Possible results?

In any measurement of the observable A associated with operator $\hat{A}$, the only values that will ever be observed are the eigenvalues of $\hat{A}$

If the particle, before the measurement, is in an eigenstate $\psi_\alpha(x)$ of $\hat{A}$ then the result is with certainty the eigenvalue a_α

If the particle, before the measurement, is in whatever state

$$\psi(x) = \sum_\alpha C_\alpha \psi_\alpha(x) \quad \text{with} \quad \sum_\alpha |C_\alpha|^2 = 1$$

Then the result is randomly an eigenvalue of the set of a_α

What is the corresponding probability law?

We know that $\langle a \rangle = \int \psi^* [\hat{A}\psi] \, dx = \ldots = \sum_\alpha |C_\alpha|^2 \, a_\alpha$

$$\langle a^n \rangle = \int \psi^* [\hat{A}^n \psi] \, dx = \ldots = \sum_\alpha |C_\alpha|^2 \, a_\alpha^n$$

leading to the probability law $a_\alpha : p_\alpha = |C_\alpha|^2$

3^{rd} postulate (strong version)

In any measurement of the observable A associated with operator $\hat{A}$, the only values that will ever be observed are the eigenvalues, which satisfy the eigenvalue equation

$$\hat{A}\psi_\alpha(x) = a_\alpha\,\psi_\alpha(x)$$

a_α Eigenvalue (non-degenerate)

$\psi_\alpha(x)$ Orthonormal eigenfunctions

Before the measurement: $\psi(x) = \sum_\alpha C_\alpha \psi_\alpha(x)$ with $\sum_\alpha |C_\alpha|^2 = 1$

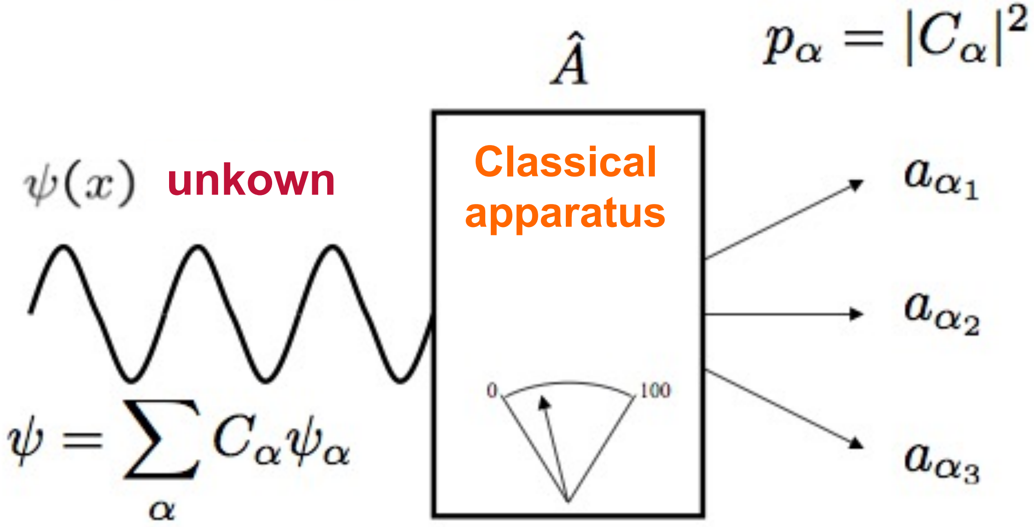
(a) If the system is in an eigenstate of $\hat{A}$ with eigenvalue a_α then any measurement of the quantity will yield a_α

(b) The probability that eigenvalue a_α will occur -- it is the absolute value squared of the coefficient, $p_\alpha = |C_\alpha|^2$

(c) After measurement of $\psi(x)$ yields some eigenvalue a_α, the wave function immediately collapses into the corresponding eigenstate $\psi_\alpha(x)$. In the case that is degenerate, $\psi(x)$ becomes the projection of $\psi(x)$ onto the degenerate subspace associated to the eigenvalue a_α

What to learn from a measurement?

A single measurement performed on a single particle reveals information on the state of the quantum system after the measurement



If the result is α_2 the state immediately after is

$$\psi = \psi_{\alpha_2}$$

From this single measurement, we cannot retrieve the state $\psi(x)$

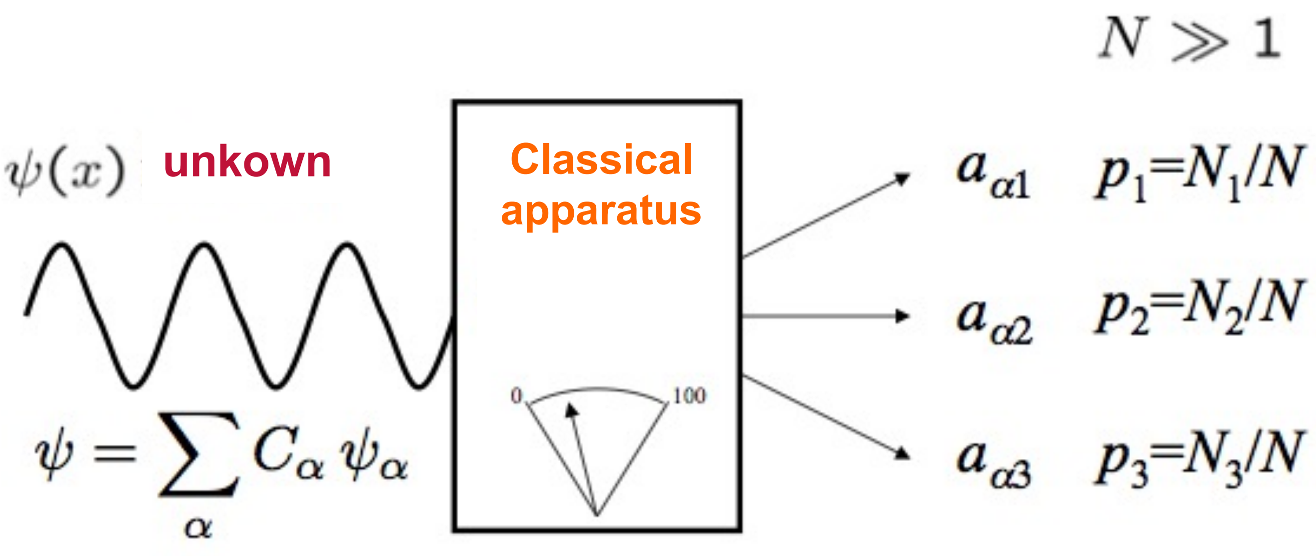
We only know that $p_{\alpha 2}$ is not zero

The wave function is modified in an irreversible way by the measurement

Wave function collapse e.g. quantum decoherence

What to learn from a measurement?

If we prepare N particles in the same quantum state (unknown), it is possible to determine the probabilities p_α. This would require to perform only a single measurement of A on each particle



From $p_\alpha = |C_\alpha|^2$ it is possible to retrieve at least partially $\psi(x)$

4.

Eingenstates of the Hamiltonian &

Resolution of the Schrödinger equation

Evolution of an eigenstate

We determine the eigenstates of the Hamiltonian $\hat{H}\psi_n(x) = E_n\,\psi_n(x)$

The set of functions ψ_n **is an orthonormal basis of wave functions**

Initial wave function: $\psi(x,0) = \sum_n C_n\,\psi_n(x)$ **with** $C_n = \int \psi_n^*(x)\psi(x,0)dx$

Wave function at time t: $\psi(x,t) = \sum_n C_n\,\psi_n(x)\,e^{-iE_nt/\hbar}$

Proof

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\,\psi(x,t)$$

$$i\hbar\frac{\partial\psi}{\partial t} = i\hbar\sum_n C_n\psi_n(x)\left(\frac{-iE_n}{\hbar}\right)e^{-iE_nt/\hbar} = \sum_n C_nE_n\psi_n(x)\,e^{-iE_nt/\hbar}$$

$$\hat{H}\,\psi(x,t) = \sum_n C_n\hat{H}\,\psi_n(x)e^{-iE_nt/\hbar} = \sum_n C_nE_n\psi_n(x)\,e^{-iE_nt/\hbar}$$

QED

Eigenstates of the Hamiltonian

Consider the particle in the initial state at t=0 $\psi(x,0) = \psi_n(x)$ Wave packet collapse

Then, the solutions of the Schrödinger equation at time t is given by

$$\psi(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$$

The eigenstates of the Hamiltonian are stationary states

→ the probability density is time independent $|\psi(x,t)|^2 = |\psi_n(x)|^2$

Also valid for all expected values associated to any physical quantities

$$\begin{aligned}\langle a\rangle(t) &= \int \psi^*(x,t)[\hat{A}\psi(x,t)]\, dx \\ &= \int \psi_n^*(x)[\hat{A}\psi_n(x)]\, dx\end{aligned}$$

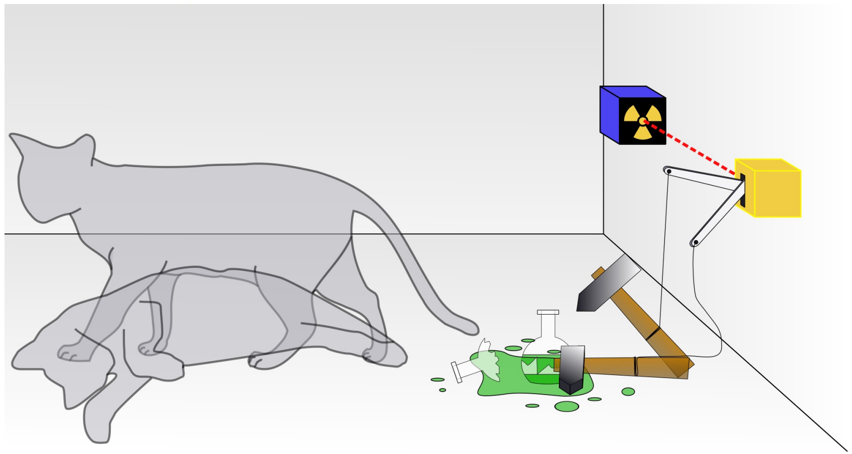
No time dependence!

Schrödinger's cat

A diabolic trap: A cat, a flask of poison, and a radioactive source are placed in a sealed box! If an internal monitor (e.g. Geiger counter) detects radioactivity (i.e. a single atom decaying), the flask is shattered, releasing the poison, which kills the cat!

The principle of superposition tells that the cat is both dead and alive e.g. the cat is in a superposition of different states

$$\psi = \frac{1}{\sqrt{2}}[\psi_{alive} + \psi_{dead}]$$



Which state for the cat?
Was it a stupid question?

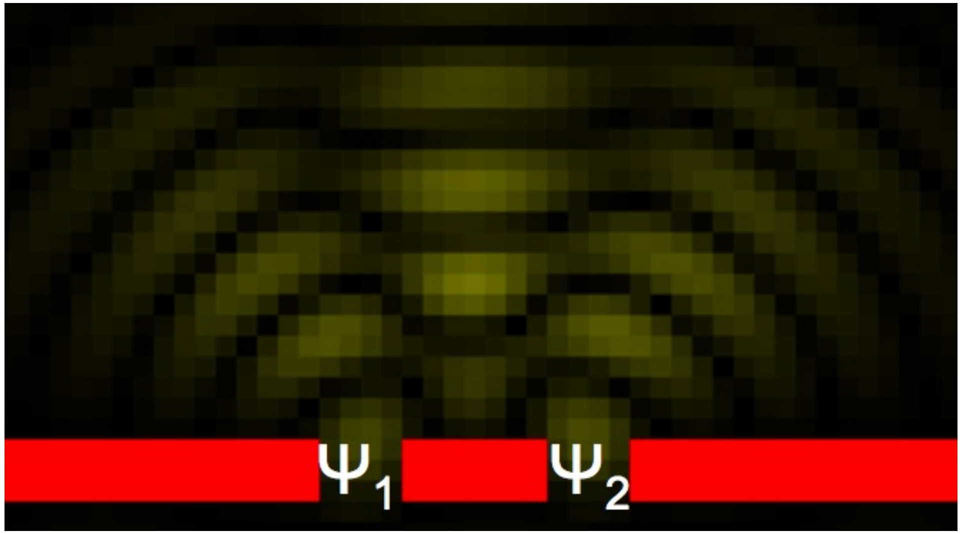
Schrödinger's cat in the garden of the Zu Vier Wachten (Zürich). Depending on the light conditions, the cat appears either alive or dead.

Schrödinger's cat

NO because a quantun system is in a superposition of different states

Remember the double-sit particle experiments. Which way?

$$\psi = \frac{1}{\sqrt{2}}[\psi_1 + \psi_2]$$



Schrödinger's cat brings the following question: Can we observe macroscopic quantum states superposition? We also see that this thought experiment contains the concept of entanglement (i.e. cat/atom, photon/slits)

Schrödinger's cat

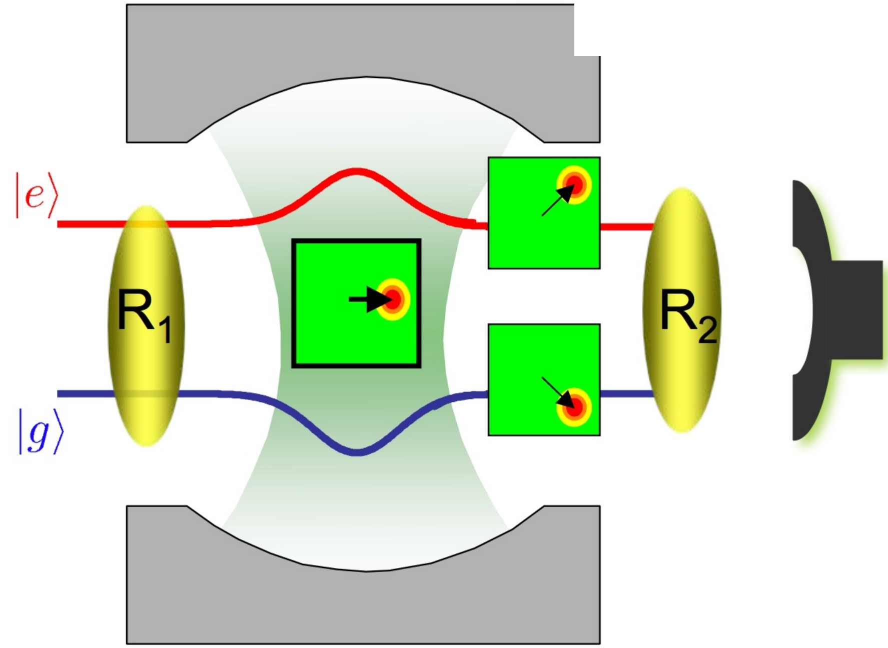
PHYSICAL REVIEW A VOLUME 45, NUMBER 7 1 APRIL 1992

Manipulation of photons in a cavity by dispersive atom-field coupling: Quantum-nondemolition measurements and generation of "Schrödinger cat" states

M. Brune, S. Haroche, and J. M. Raimond
Laboratoire de Spectroscopie Hertzienne de l'Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris CEDEX 05, France

The Nobel Prize in Physics 2012
Serge Haroche, David J. Wineland

Rydberg's atoms

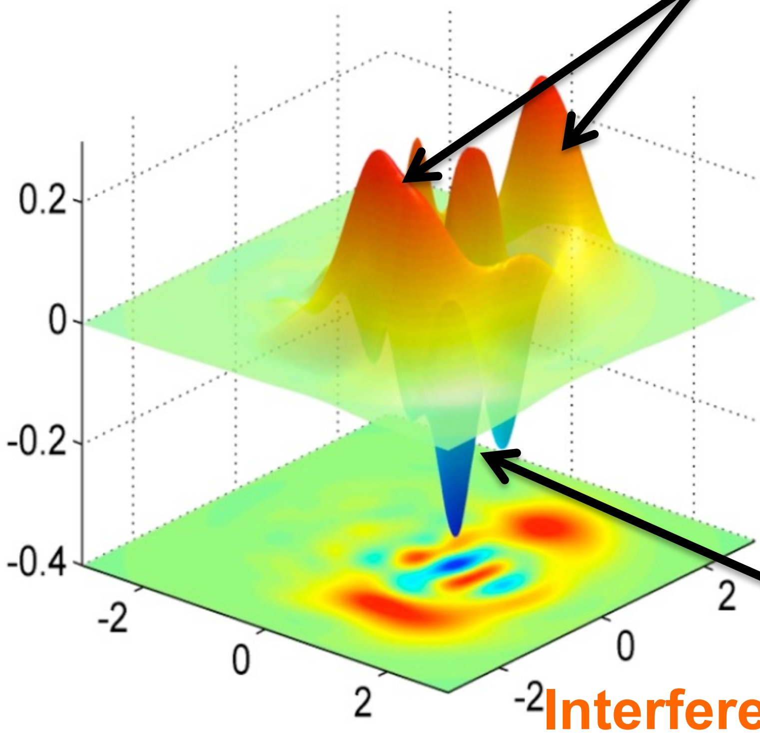


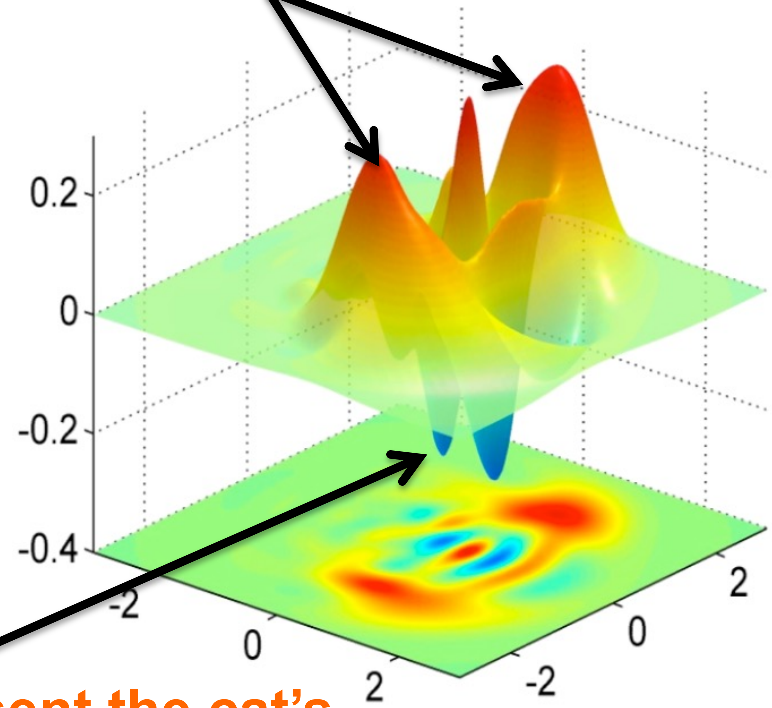
S. Deléglise et al, Nature, vol. 455, pp. 510 (2008)

Schrödinger's cat

By producing quantum interferences, it is possible to show that a "AND" in quantum mechanics can be transformed into a "OR" in classical physics (quantum decoherence)

Quantum states: cat "dead" or "alive"



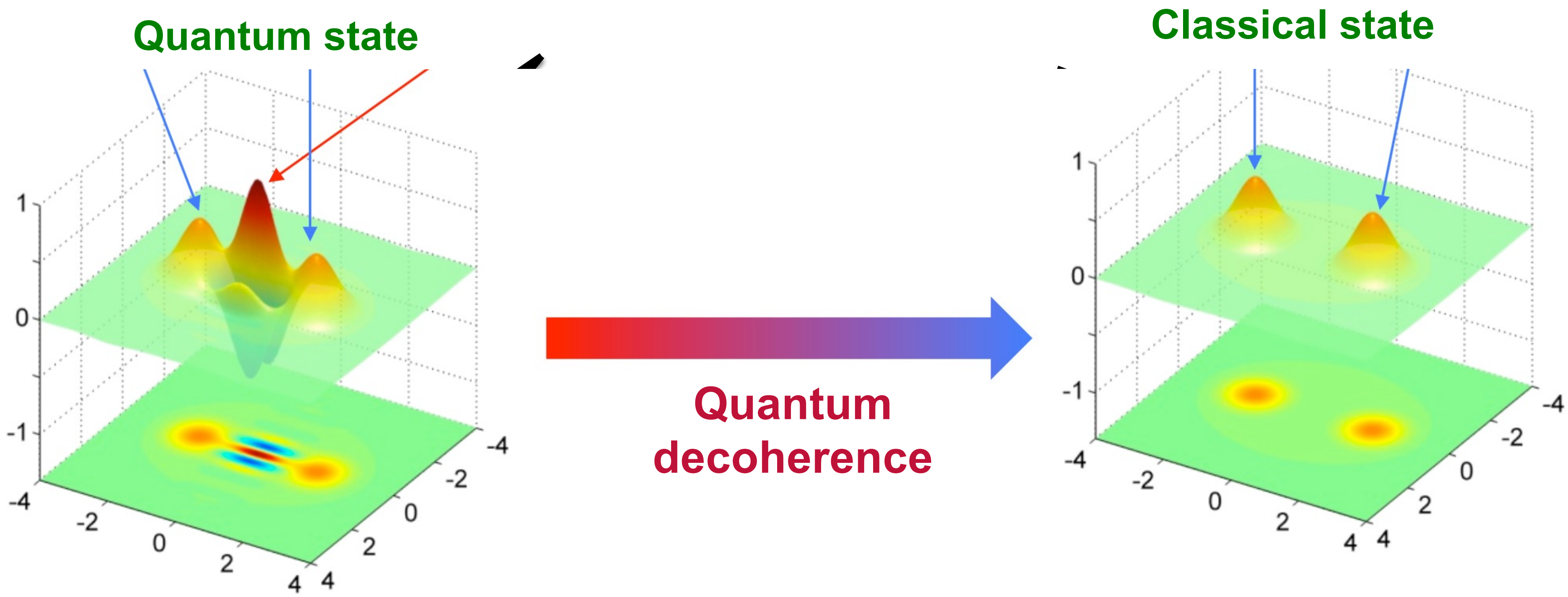


Interferences represent the cat's quantum coherence

S. Deléglise et al, Nature, vol. 455, pp. 510 (2008)

Schrödinger’s cat

By producing quantum interferences, it is possible to show that a “AND” in quantum mechanics can be transformed into a “OR” in classical physics (quantum decoherence)

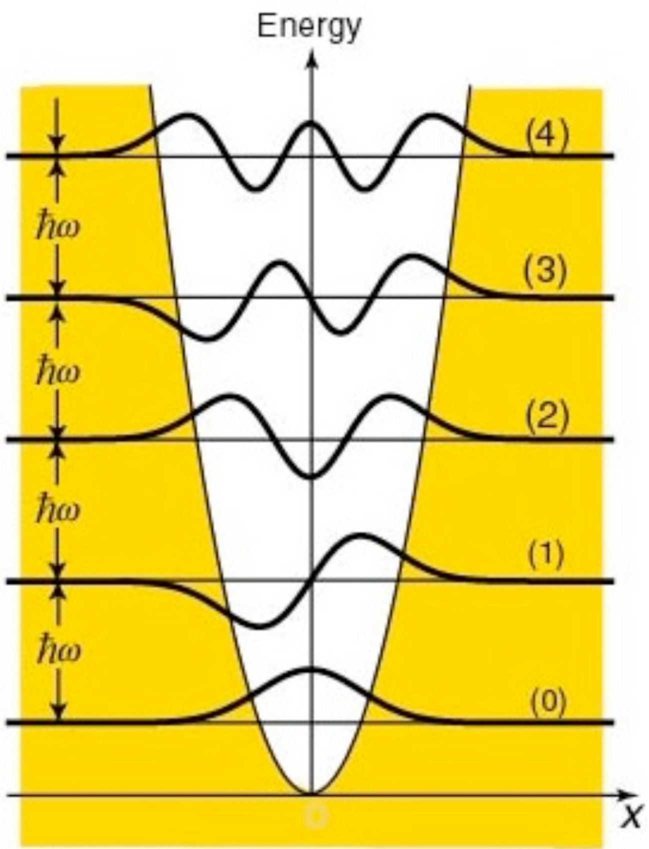


Classical-quantum limit: objects with large number of particles does not see any superposition i.e. the time for quantum decoherence is ultrafast and scales with the number of particles

Superposition & quantum decoherence

Section 4

The Quantum Harmonic Oscillator*



Dirac's notations used in this section are explained in section 6

What we know from classical mechanics

The simple harmonic oscillator describes linear, undamped oscillatory dynamics like mass-spring systems, vibration of molecules, LC circuits, etc

$$m\frac{d^2x}{dt^2} = -Kx = -m\omega^2 x$$

The force needed to extend or compress a spring by some distance is proportional to that distance

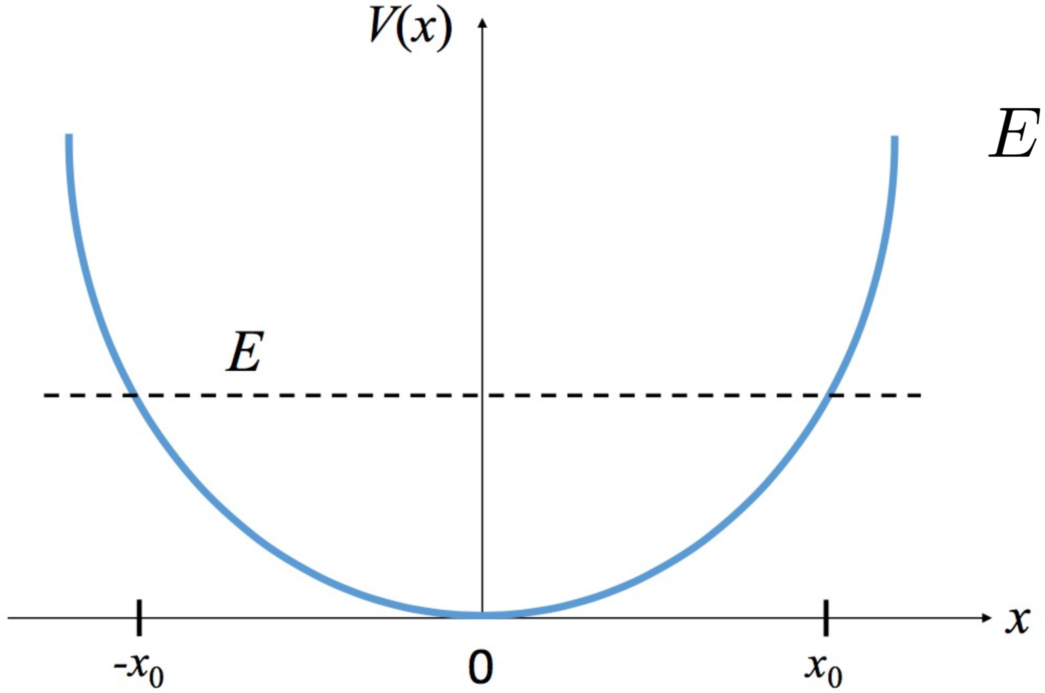
Potential energy $$V(x) = \frac{Kx^2}{2} = \frac{m\omega^2 x^2}{2}$$

Classical solutions

$$x(t) = A\cos(\omega t + \delta)$$
$$p(t) = -mA\omega\sin(\omega t + \delta)$$

What we know from classical mechanics

The total energy of this system is conserved and oscillates between kinetic and potential



$$E = \frac{1}{2}mv^2 + \frac{1}{2}Kx^2 = \text{constant}$$

Turning points

$$x_0 = \pm\sqrt{\frac{2E}{m\omega^2}}$$

Now let us move to the quantum harmonic oscillator which is useful to explain the quantization of the electromagnetic field, and oscillations of the certain molecules like NH_3

Quantum harmonic oscillator

Consider the Hamiltonien

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{x}^2$$

And the following operators

Annihilation or lowering operator $\hat{a} \equiv \hat{a}_- = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$

Creation or raising operator $\hat{a}^\dagger \equiv \hat{a}_+ = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$

We can rewrite,

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger) \quad \textbf{and} \quad \hat{p} = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger)$$

leading to $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$

Quantum harmonic oscillator

The Hamiltonian can be written as

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$$

with $\hat{N} = \hat{a}^\dagger \hat{a}$ **the "Number operator" (Hermitian)**

Commutation relationships

$$[\hat{x}, \hat{p}] = i\hbar \quad [\hat{a}, \hat{a}^\dagger] = 1 \quad [\hat{N}, \hat{a}] = -\hat{a} \quad [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$$

We can demonstrate that the eigenstates of $\hat{H}$ are also eigenstates of $\hat{N}$

Eigenvalue equation $\hat{N}\,|n\rangle = n\,|n\rangle$ $\quad n$ **are real eigenvalues**

Quantum harmonic oscillator

Since we have proved that $\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$

the energy eigenvalue corresponding to state $|n\rangle$ is defined as follows

$$E_n = (n + \tfrac{1}{2})\hbar\omega \text{ for } n = 0, 1, 2, \ldots .$$

We can also observe that,

$\hat{a}^\dagger |n\rangle \ (\hat{a}|n\rangle)$ is an eigenfunction of $\hat{H}$ and $\hat{N}$

$$\hat{N}\hat{a}^\dagger |n\rangle = ([\hat{N}, \hat{a}^\dagger] + \hat{a}^\dagger \hat{N}) |n\rangle = (n+1)\hat{a}^\dagger |n\rangle$$

$$\hat{N}\hat{a} |n\rangle = ([\hat{N}, \hat{a}] + \hat{a}\hat{N}) |n\rangle = (n-1)\hat{a} |n\rangle$$

$\hat{a}^\dagger \ (\hat{a})$ "creates" ("annihilates") one unit $\hbar\omega$ of energy

Quantum harmonic oscillator

$$\hat{N}\hat{a}\,|n\rangle = (n-1)\hat{a}\,|n\rangle \quad \Rightarrow \quad \hat{a}\,|n\rangle = c\,|n-1\rangle$$

Assuming $|n\rangle$ **is normalized, we get** $\langle n|n\rangle = 1$

$$\langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = |c|^2 \text{ and } \langle n|\hat{a}^{\dagger}\hat{a}|n\rangle = \langle n|\hat{N}|n\rangle = n$$

$\Rightarrow$ $n = |c|^2$ $\Rightarrow$ **This means that** n **must be real and nonnegative**

Then we end up with the following relations

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \text{ and } \hat{a}^{\dagger}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

Quantum harmonic oscillator

Let us apply $(\hat{a})$ sequentially to an eigenstate $|n\rangle$

$$\hat{a}^2\,|n\rangle = \sqrt{n(n-1)}\,|n-2\rangle$$

$$\hat{a}^3\,|n\rangle = \sqrt{n(n-1)(n-2)}\,|n-3\rangle$$

$$\vdots$$

If n is a positive integer, this sequence must terminate when we get to $\sqrt{n(n-1)\ldots 0}$

If n is not a integer, then the sequence won't terminate since n can be negative. But we proved all n are positive

Ergo, the sequence terminates at $n = 0$ and n in general must be a nonnegative integer $(n = 0, 1, 2, \ldots)$

Quantum harmonic oscillator

We can construct the form of the eigenstates $|n\rangle$ in Hilbert space using $\hat{a}^\dagger$ if we know $|0\rangle$

$$|1\rangle = \hat{a}^\dagger |0\rangle$$

$$|2\rangle = \frac{\hat{a}^\dagger}{\sqrt{2}} |1\rangle = \frac{(\hat{a}^\dagger)^2}{\sqrt{2}} |0\rangle$$

$$|3\rangle = \frac{\hat{a}^\dagger}{\sqrt{3}} |2\rangle = \frac{(\hat{a}^\dagger)^3}{\sqrt{3!}} |0\rangle$$

$$\vdots$$

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$$

Quantum harmonic oscillator

If we move back to the x-representation

$$\hat{a}\,|0\rangle = 0 \quad \Rightarrow \quad \langle x'|\hat{a}|0\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left\langle x' \middle| \hat{x} + \frac{i\hat{p}}{m\omega} \middle| 0 \right\rangle$$

with $x_0 = \sqrt{\dfrac{\hbar}{m\omega}}$

$$= \left(x' + x_0^2 \frac{d}{dx'}\right)\langle x'|0\rangle = 0$$

The normalized solution to this differential equation is Gaussian

$$\psi_0(x') = \langle x'|0\rangle = \frac{1}{\pi^{1/4}\sqrt{x_0}} \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

Quantum harmonic oscillator

For n >0, we can construct $|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$

In general, we have

$$\psi_n(x') = \langle x'|n\rangle = \frac{1}{\pi^{1/4} x_0^{n+1/2} \sqrt{2^n n!}} \left(x' - x_0^2 \frac{d}{dx'}\right)^n \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

Polynomial expression

$$\psi_n(x') = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} \mathcal{H}_n\left(\frac{x'}{x_0}\right) \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right]$$

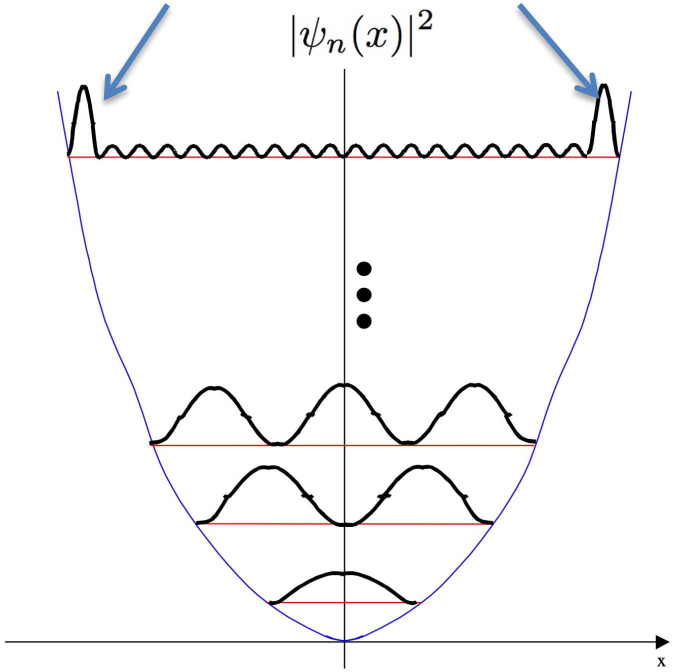
$\mathcal{H}_n(z)$ Hermite polynomials such that

$$\mathcal{H}_1(z) = 2z,\ \mathcal{H}_2(z) = 4z^2 - 2,\ \text{etc.}$$

Further readings: Arfken and Weber, Mathematical Methods for Physicists, Academic Press, Wiley

Quantum harmonic oscillator

Large n → classical case



Classical mechanics

$$E = \frac{1}{2}m\omega^2 x_0^2 \qquad x_0 = \pm\sqrt{\frac{2E}{m\omega^2}}$$

Quantum mechanics

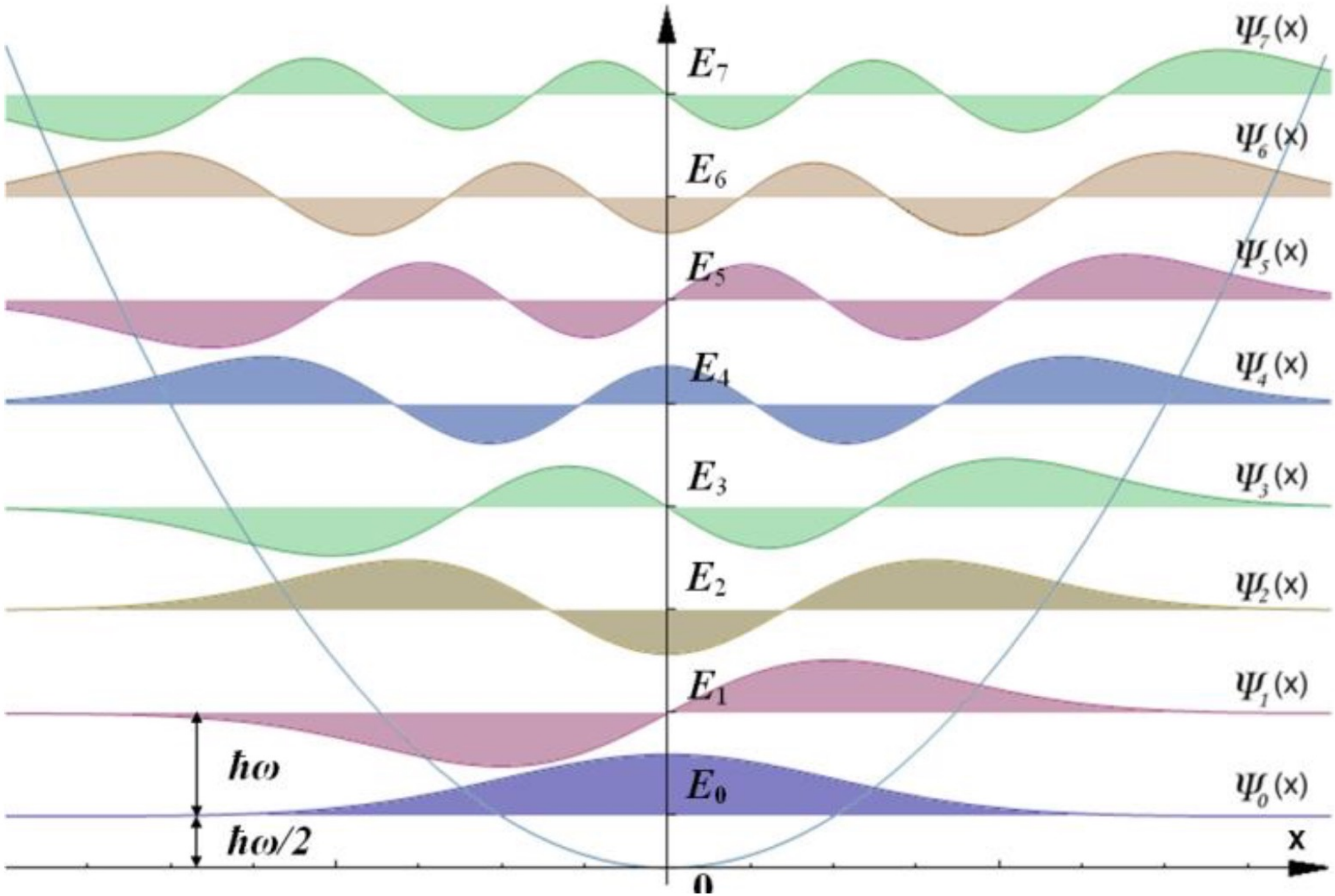
$$E_n = (n+\tfrac{1}{2})\hbar\omega \qquad x_0^2 = \frac{2\hbar\omega(n+\frac{1}{2})}{m\omega^2}$$

The ground state (lowest energy eigenstate) has energy $E_0 = \hbar\omega/2$ (zero point energy)

The set of energy E_n is discrete (bound states) and evenly spaced

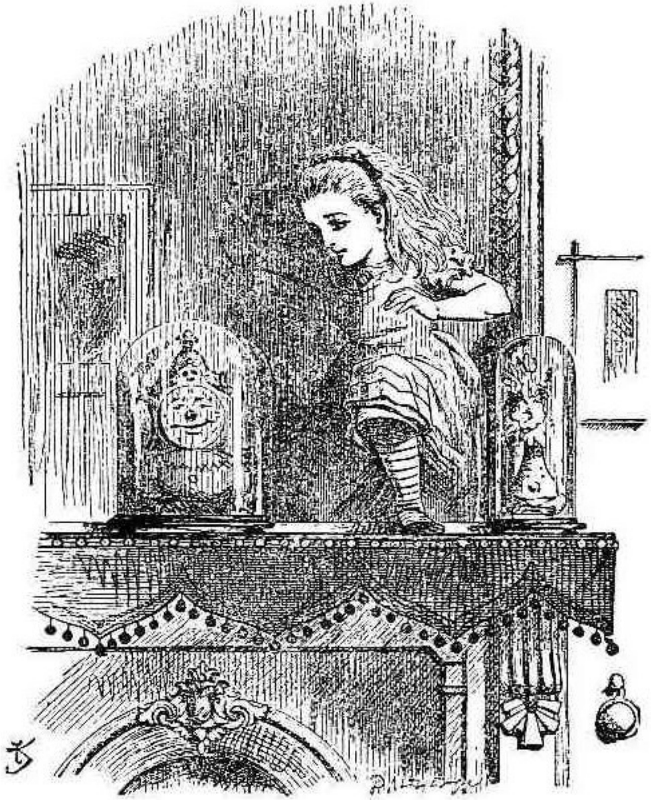
We define $\hat{a}\,|0\rangle = 0$ e.g. applying $\hat{a}$ to the lowest energy eigenstate destroys the state

$$E_n = (n + \frac{1}{2})\hbar\omega \text{ for } n = 0, 1, 2 \ldots$$



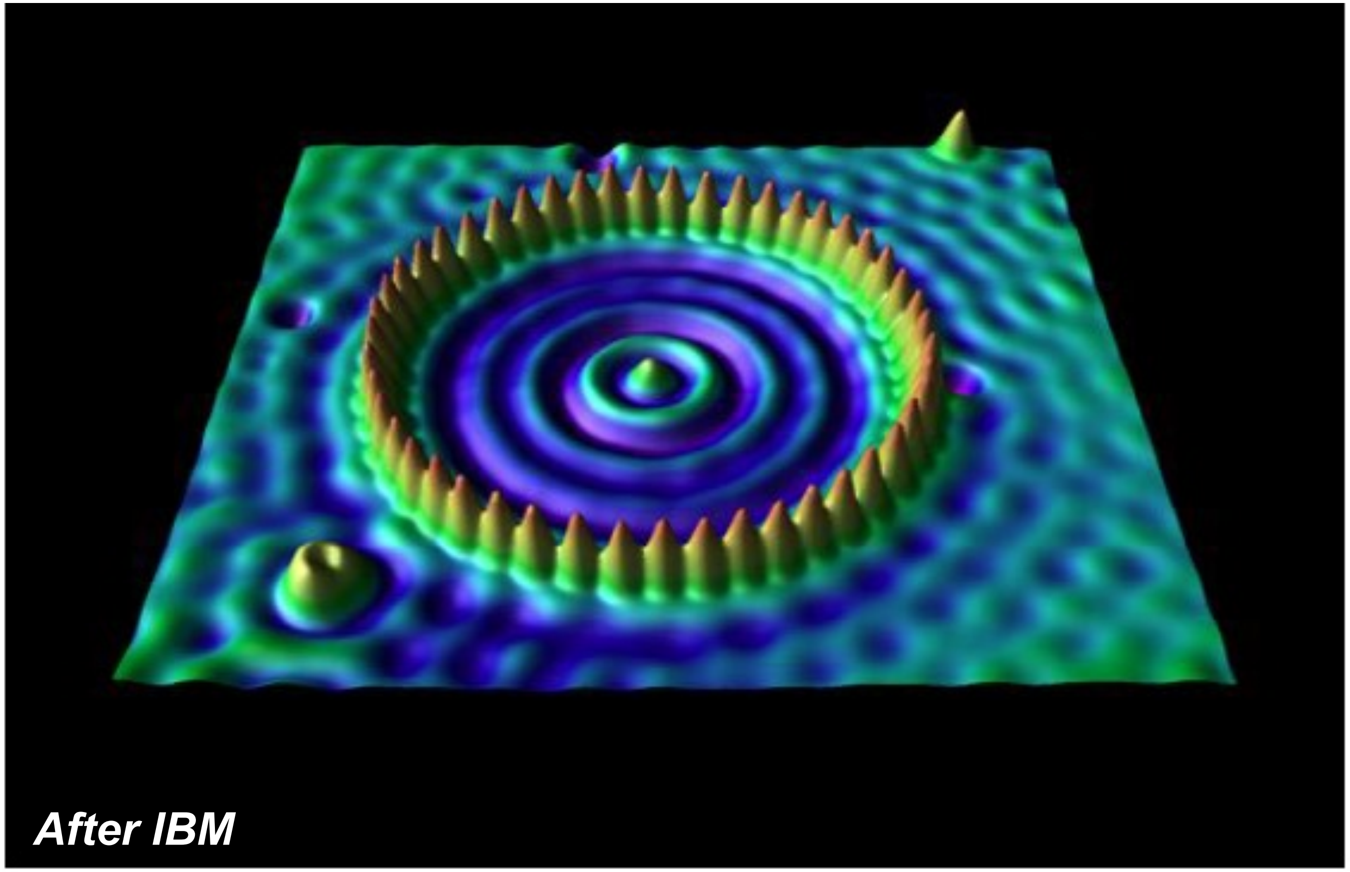
Section 5

Quantization of Simple Physical Systems



Alice going thru a looking glass, After Lewis Carroll

Quantum corral reef



Scanning tunneling microscopy: this image shows 48 iron atoms positioned into a circular ring. The ripples in the ring of atoms are the wave patterns of some of the electrons that were trapped in the corral

1.
Bound and scattering states

Reminders

Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$

Search the eingenstate of the Hamiltonian $\hat{H}\psi_\alpha(x) = E_\alpha\,\psi_\alpha(x)$

E_α **Real eingenvalue (energy)**

→ Time independent Schrödinger's equation

Once we know $\psi_\alpha(x)$ **we can calculate the evolution of** $\psi(x,t)$

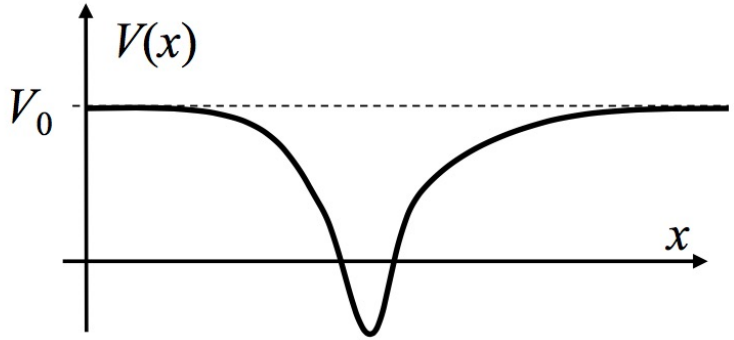
$$\psi(x,0) = \sum_\alpha C_\alpha\,\psi_\alpha(x) \quad \Longrightarrow \quad \psi(x,t) = \sum_\alpha C_\alpha\,\psi_\alpha(x)\,e^{-iE_\alpha t/\hbar}$$

→ Time evolution of the wave function state

Bound & scattering states

Consider a potential which tends to V_0 when $x \to \infty$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)$$



Two interesting cases

$\psi(x)$ **goes to 0 when x → ∞**

If $\int |\psi(x)|^2 \, \mathrm{d}x = 1$ **State eligible as a wave function**

→ bound states

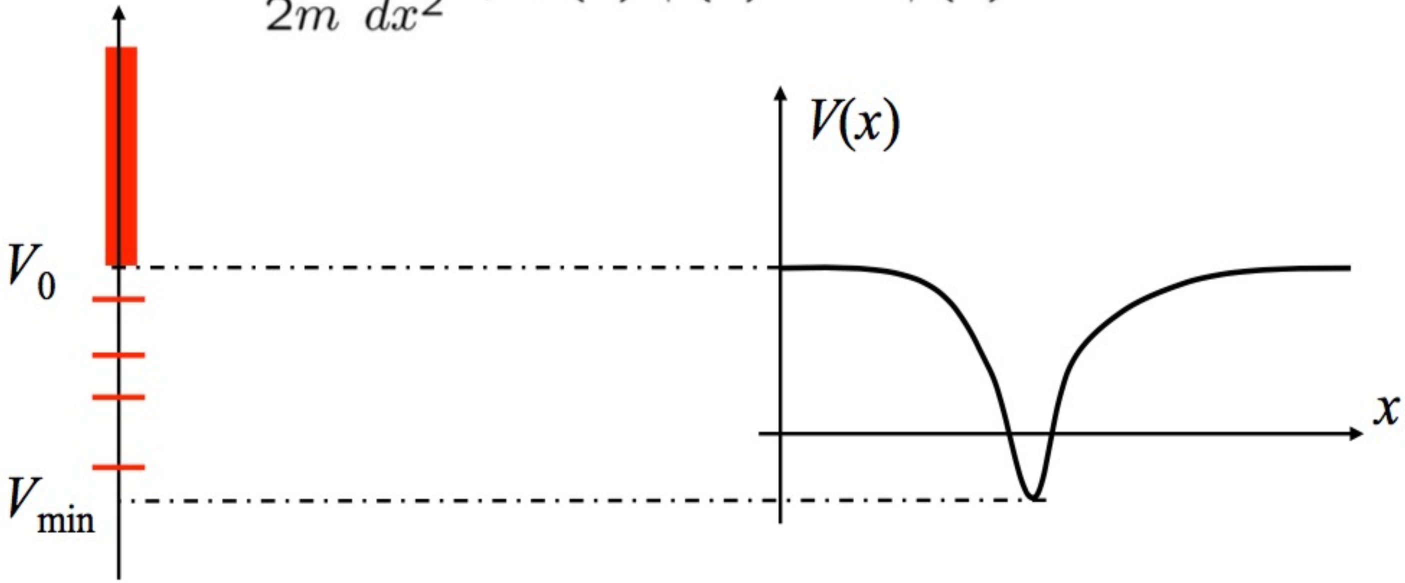
$\psi(x)$ **behaves as a combination of plane waves at infinity**

$\psi(x) \simeq \alpha e^{ikx} + \beta e^{-ikx}$ **when** $x \to +\infty$ et/ou $-\infty$

Can be used to create wave packets → scattering states

Bound & scattering states

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\,\psi(x)=E\,\psi(x)$$

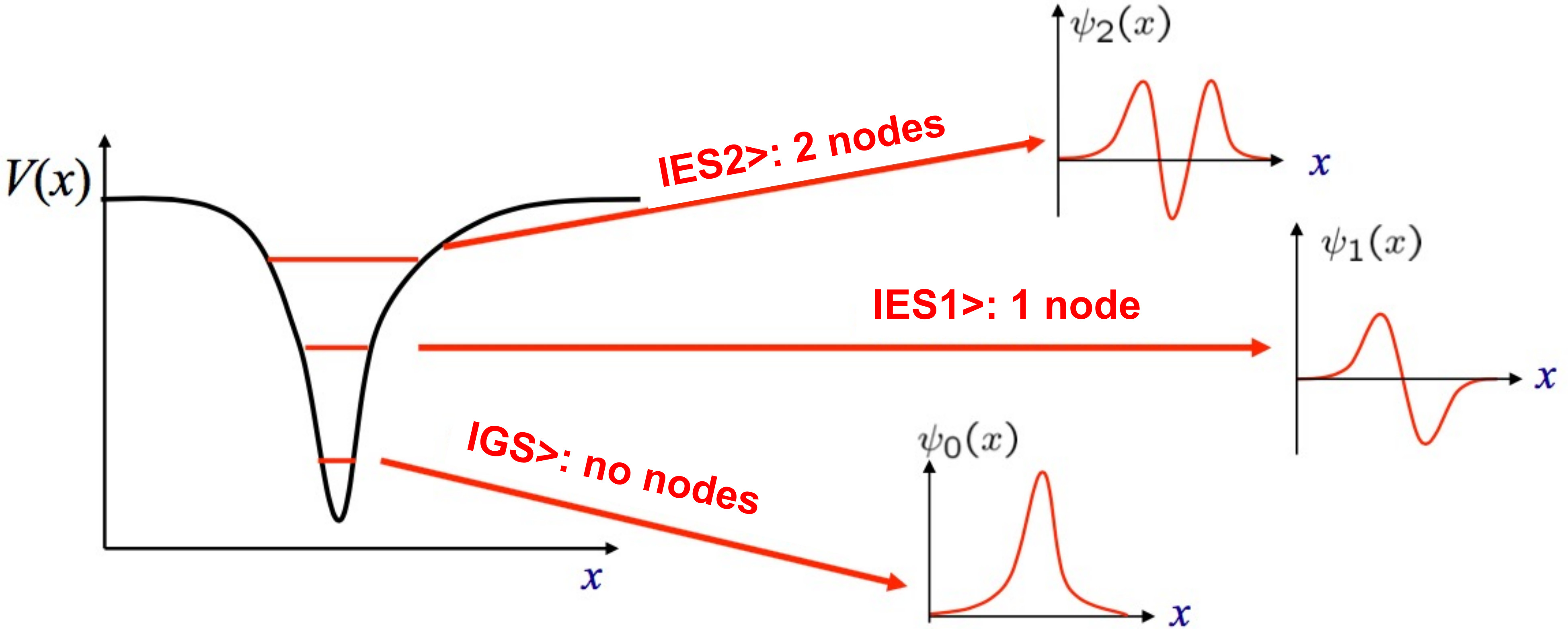


- No relevant states for $E<V_{min}$
- Between V_{min} and V_0: Bound states (finite number of elligible states)
- Beyond V_0, energy continuum: Scattering states (i.e. domain of the plane waves)

Steady-state solutions

Sturm-Liouville theorem (real wave functions): As we change to a higher energy level, the index n grows, and we have more nodes (points where the sign changes) of the wave function

Further readings: Arfken and Weber, Mathematical Methods for Physicists, Academic Press, Wiley

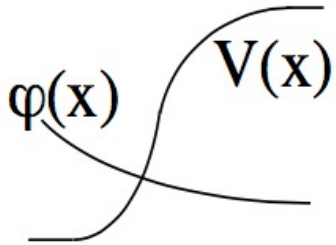


Case of symmetric potentials: Odd or even eigenfunctions (nondegenerate) or whatever (degenerate)

Boundary conditions

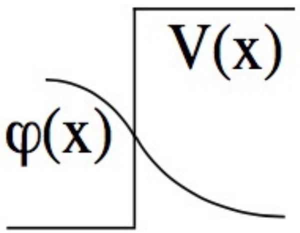
Potential V(x) | **Wave function φ(x)**

Continuous,
bounded
(real case)



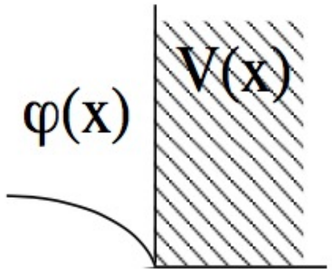
Continuous, bounded,
2nd order derivative ok

Discontinuous,
bounded
(step-like)



Continuous, bounded,
1st order derivative ok
(i.e. φ''(x) discontinuous)

Discontinuous,
unbounded
(wall-like)

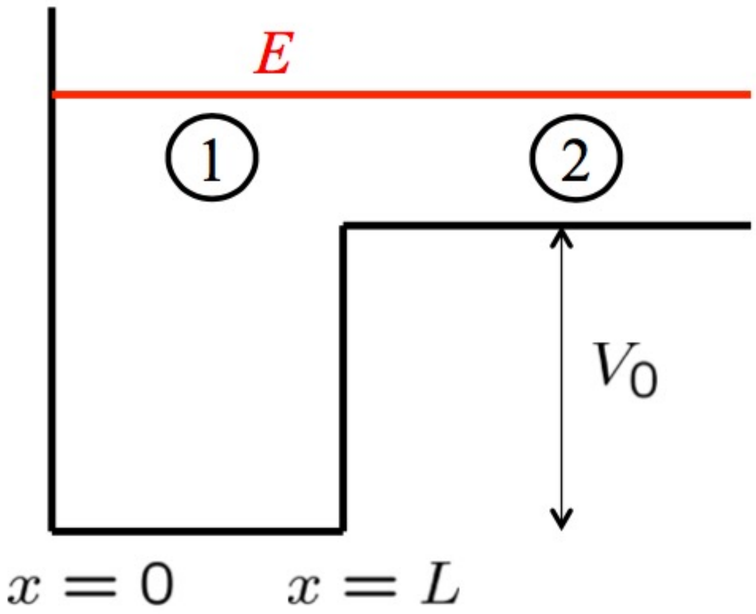


Continuous, bounded,
No derivatives
(i.e. φ'(x) discontinuous)

2.
Semi-infinite well potential

Scattering states

Consider the case with E > V_0



Region 1

$$\psi'' + k^2\psi = 0$$

$$k = \sqrt{2mE}/\hbar$$

$$\psi(0) = 0$$

$$\Rightarrow \psi(x) = A\,\sin(kx)$$

Region 2

$$\psi'' + k'^2\psi = 0$$

$$k' = \sqrt{2m(E - V_0)}/\hbar$$

$$\Rightarrow \psi(x) = B\,\sin(k'x) + C\,\cos(k'x)$$

Then, we have to write the boundary conditions at $x = L$

Scattering states

At $x = L$ the wave function ψ and its derivative ψ' are continuous

$$A\sin(kL) = B\sin(k'L) + C\cos(k'L)$$
$$kA\cos(kL) = k'\left(B\cos(k'L) - C\sin(k'L)\right)$$

$$k = \sqrt{2mE}/\hbar$$
$$k' = \sqrt{2m(E - V_0)}\,/\,\hbar$$

System of linear equations (2 equations, 3 variables) for all E>V_0

The trivial solution is $A = B = C = 0$

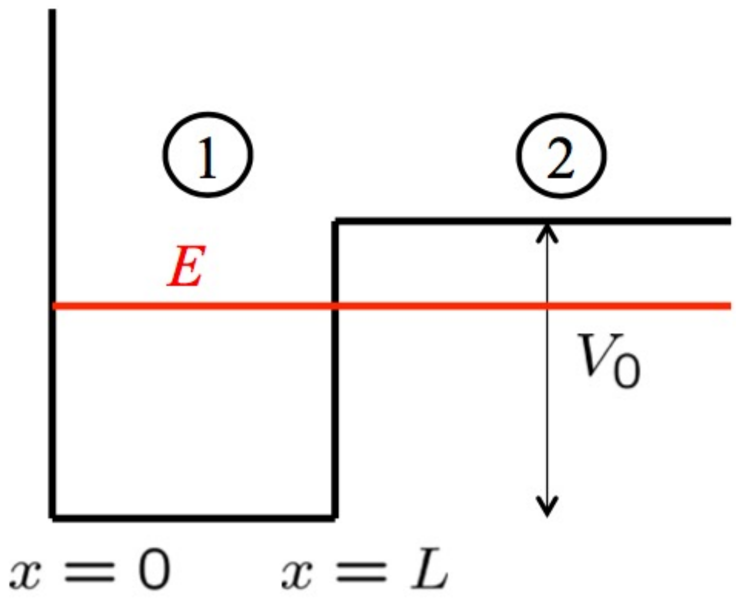
For all energies larger than the asymptotic value of the potential, we found an eigenstate ψ of the Hamiltonian. The eigenstate behaves like a plane wave at infinity

$$B\sin(k'x) + C\cos(k'x)$$

$$\Longleftrightarrow \quad \beta e^{ik'x} + \gamma e^{-ik'x}$$

Bound states

Consider the case with $E < V_0$



Region 1 $\psi'' + k^2\psi = 0$

$$k = \sqrt{2mE}/\hbar$$

$$\psi(0) = 0$$

$$\Longrightarrow \quad \psi(x) = A\sin(kx)$$

Region 2 $\psi'' - K^2\psi = 0$

$$K = \sqrt{2m(V_0 - E)}/\hbar$$

We must eliminate the term which does not have a physical meaning

$$\Longrightarrow \quad \psi(x) = B\,e^{-Kx} \cancel{+ C\,e^{Kx}}$$

Then, we have to write the boundary conditions at $x = L$

Bound states

At $x = L$ the wave function ψ and its derivative ψ' are continuous

$$A\sin(kL) = B\,e^{-KL}$$
$$kA\cos(kL) = -KB\,e^{-KL}$$

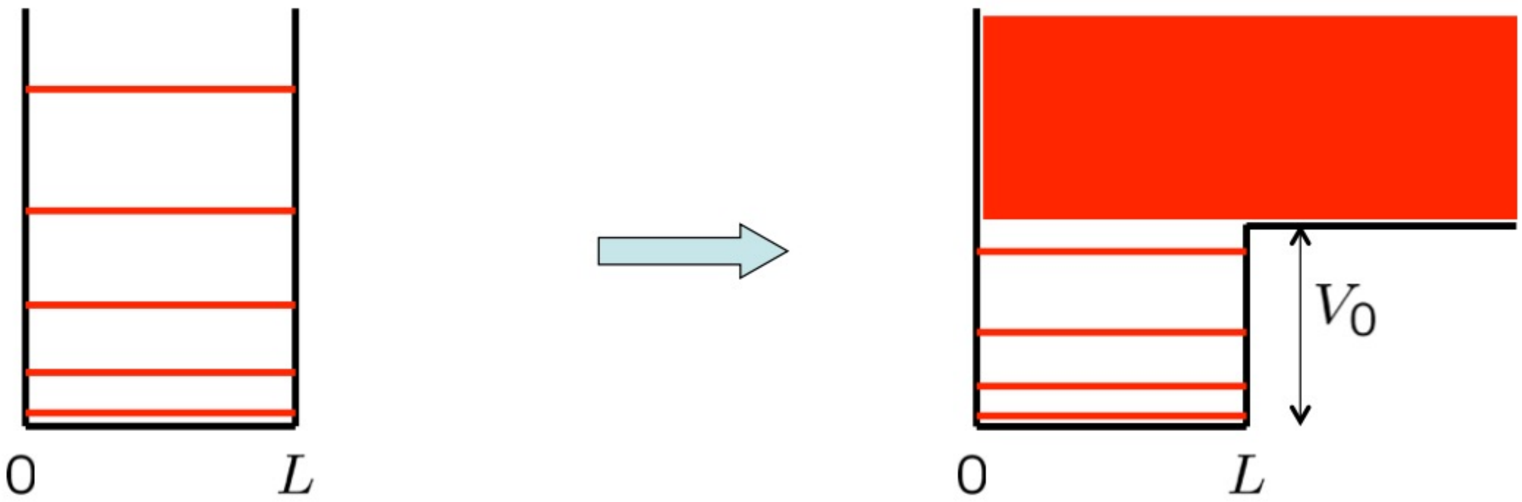
$$k = \sqrt{2mE}/\hbar$$
$$K = \sqrt{2m(V_0 - E)}\,/\,\hbar$$

System of linear equations (2 equations, 2 variables) leading to the following solution (excluding the trivial solution)

$$k\cot(kL) = -K$$

For given values of m and V_0, the above equation can only be fulfilled for discrete values of the energy E

Semi-infinite well potential

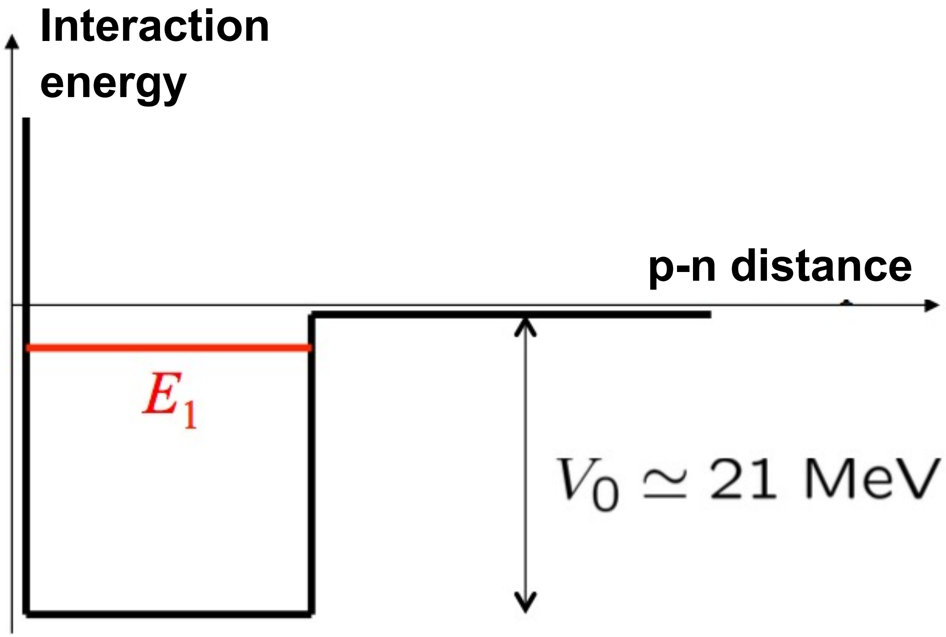


Continuum of energy states for $E > V_0$

Bound states (finite number) for $0 < E < V_0$

Example: Big-bang nucleosynthesis

Proton-neutron: 1 bound state!



$$L \simeq 2.8 \times 10^{-15} \text{ m}$$

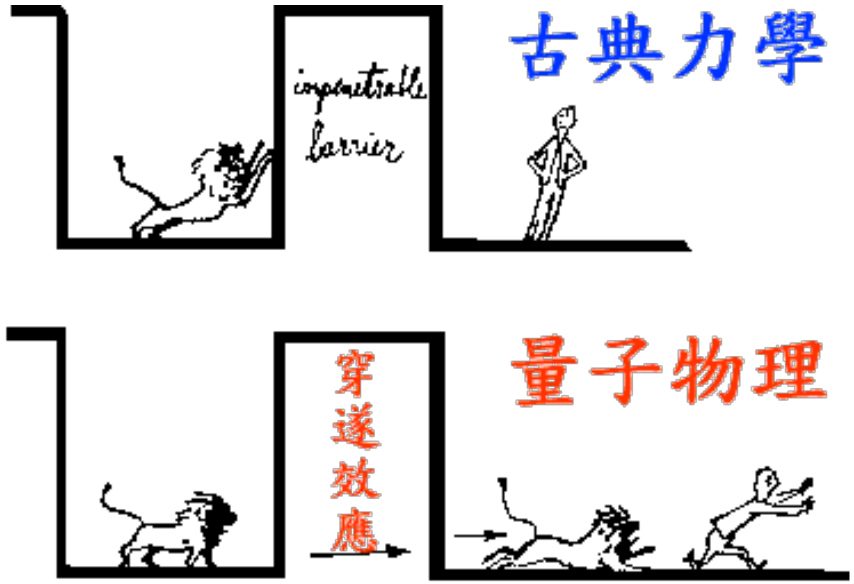
Thermonuclear reactions

$$V_0 - E_1 \simeq 2.2 \text{ MeV}$$

$$p + n \rightarrow {}^2\mathrm{H} + \gamma$$
$$p + {}^2\mathrm{H} \rightarrow {}^3\mathrm{He} + \gamma$$
$${}^2\mathrm{H} + {}^2\mathrm{H} \rightarrow {}^3\mathrm{He} + n$$
$${}^2\mathrm{H} + {}^2\mathrm{H} \rightarrow {}^3\mathrm{H} + p$$
$${}^3\mathrm{He} + {}^2\mathrm{H} \rightarrow {}^4\mathrm{He} + p$$
$${}^3\mathrm{H} + {}^2\mathrm{H} \rightarrow {}^4\mathrm{He} + n$$

Big-bang nucleosynthesis: The initial conditions (neutron-proton ratio) were set in the first second after the Big Bang → the first atoms in the Universe!

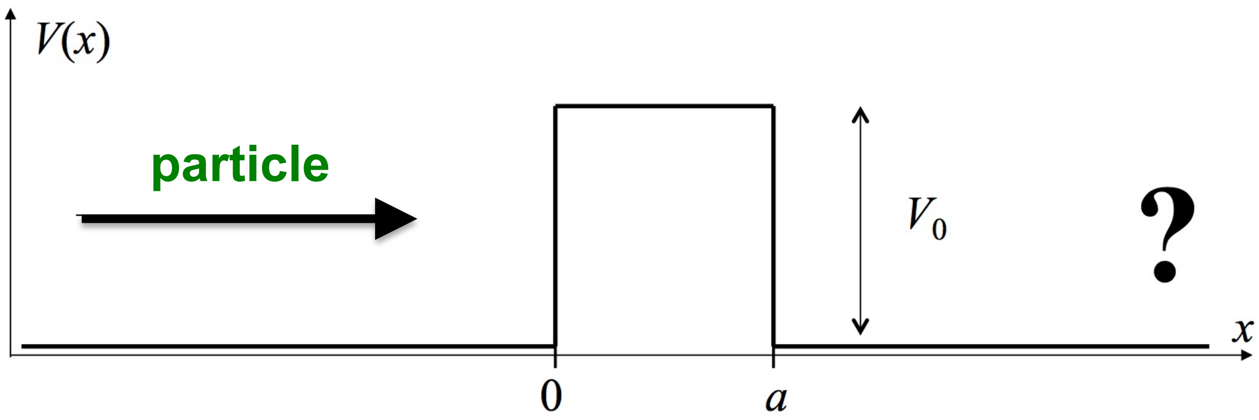
3.
Tunneling effect



The difference between classical theory and quantum theory, illustrating tunneling through potential barrier. This illustration was used by Van Vleck in his last publication, the Julian E. Mack Lecture at his Alma Mater, the University of Wisconsin, in 1979. (After B. Bleaney, Contemp. Phys. 25 (1984) 320.)

Transmission coefficient

Consider a particle with a mean energy $E<V_0$



As opposed to the classical case, quantum mechanics allows a non zero transmission coefficient that depends both on width and height of the tunnel barrier (quantum tunneling effect)

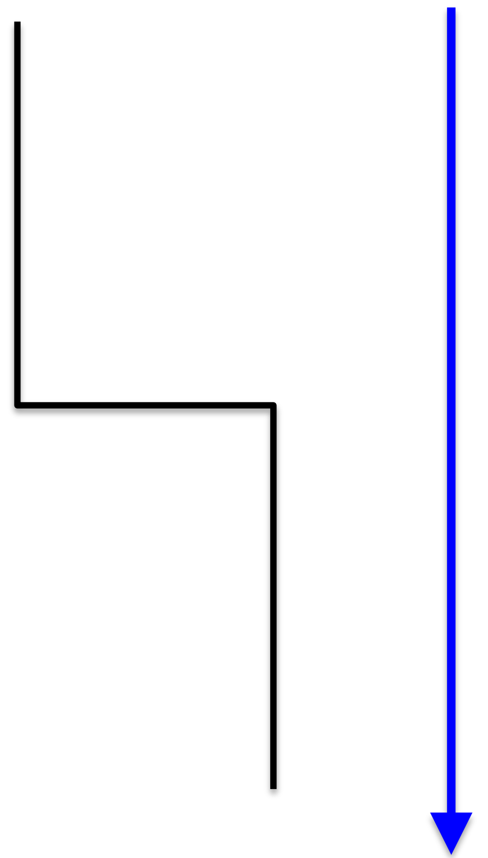
$$T \propto \exp(-2\kappa a) \qquad \kappa = \sqrt{2m(V_0 - E)}/\hbar$$

Not that this number is extremely small for macroscopic objects … at least as small as the probability to see the spontaneous flipping of a coin on a table ($10^{-1000000000000000000000000000}$)

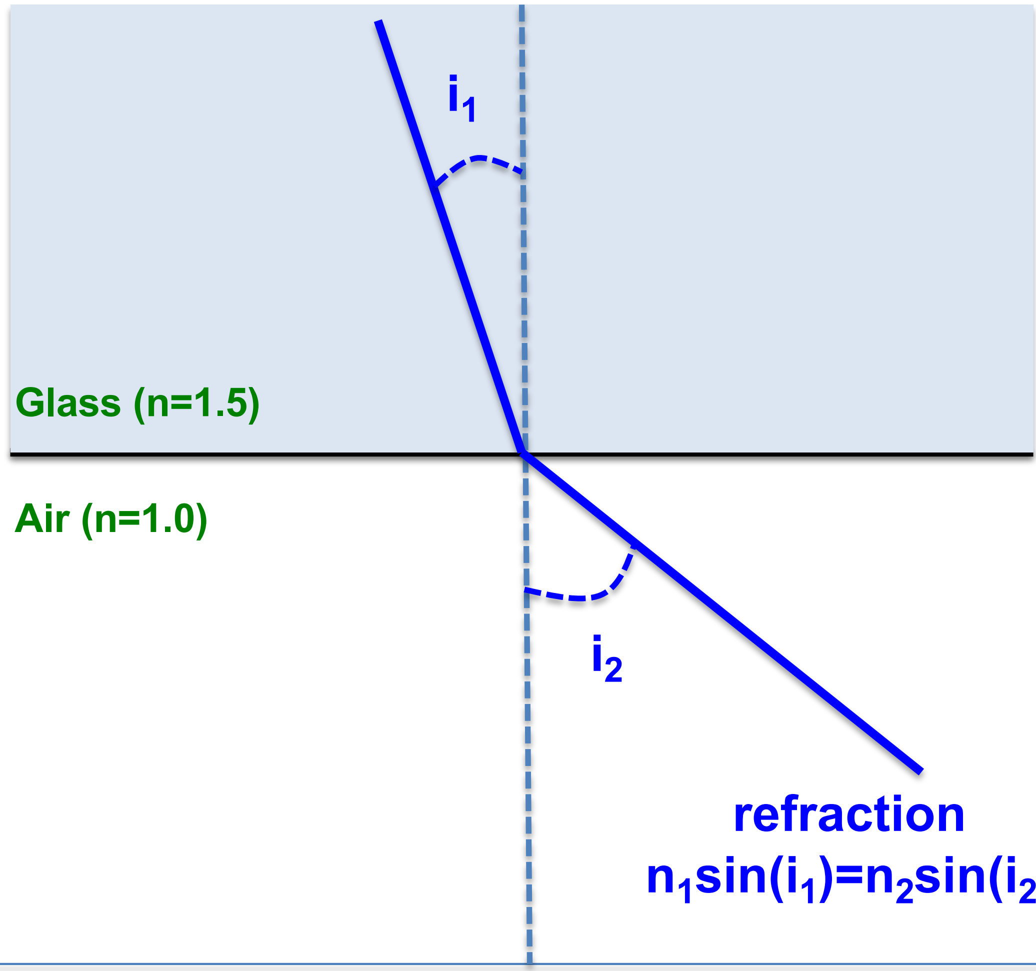
Analogy with wave optics

The tunneling effect can be simply observed in wave optics!

Potential barrier



Optical Analogy



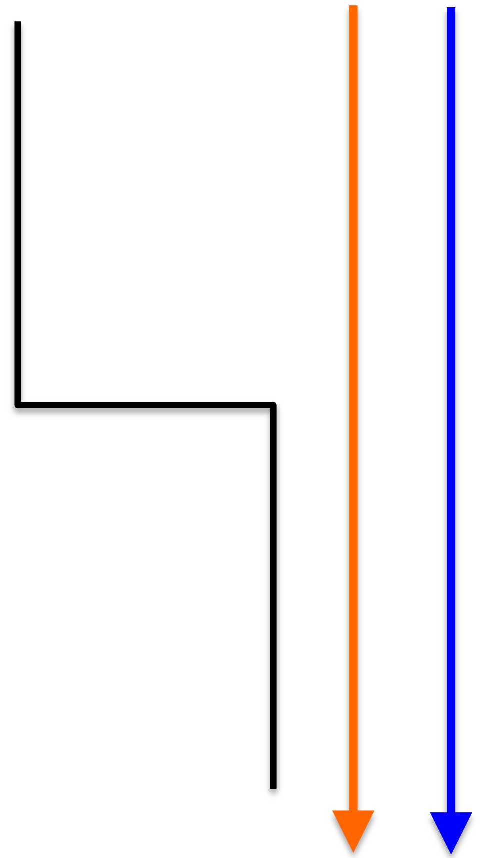
refraction

$n_1\sin(i_1)=n_2\sin(i_2)$

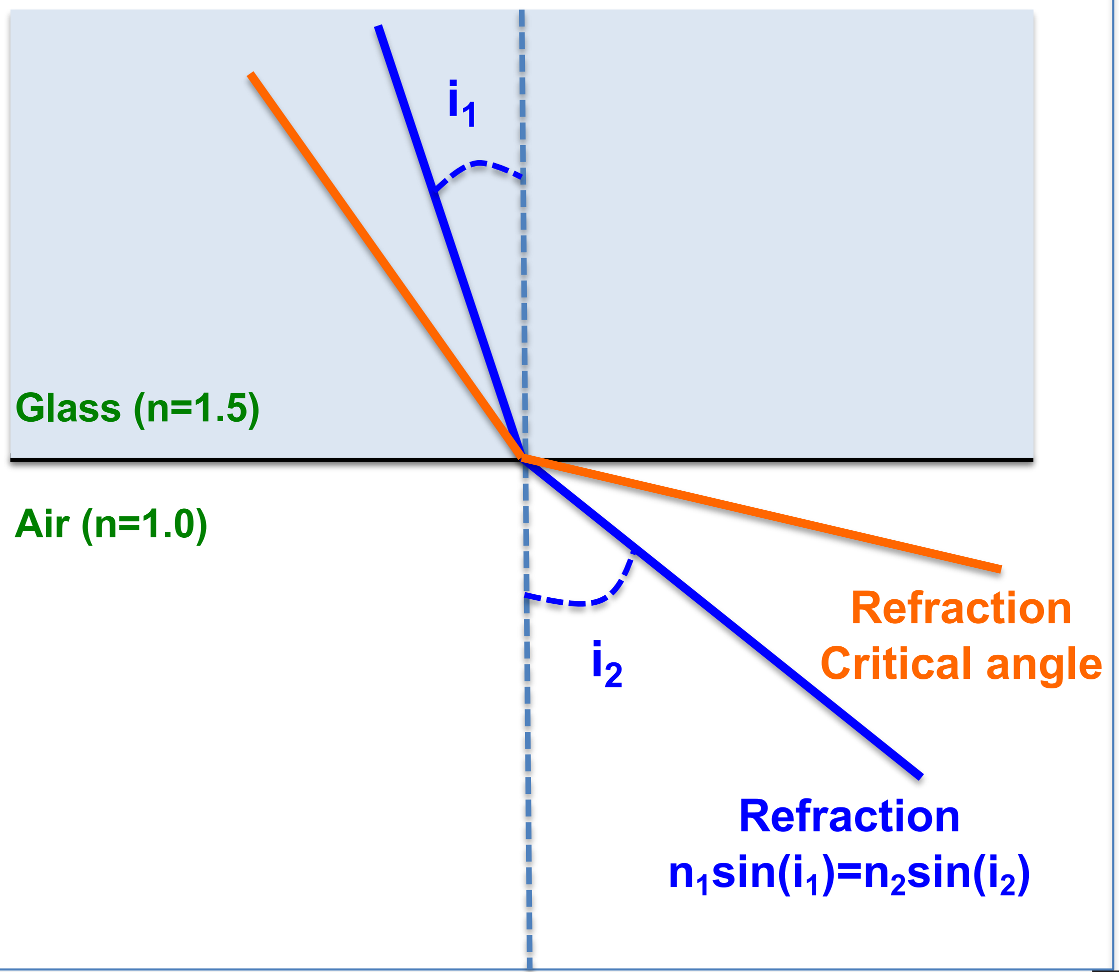
Analogy with wave optics

The tunneling effect can be simply observed in wave optics!

Potential barrier



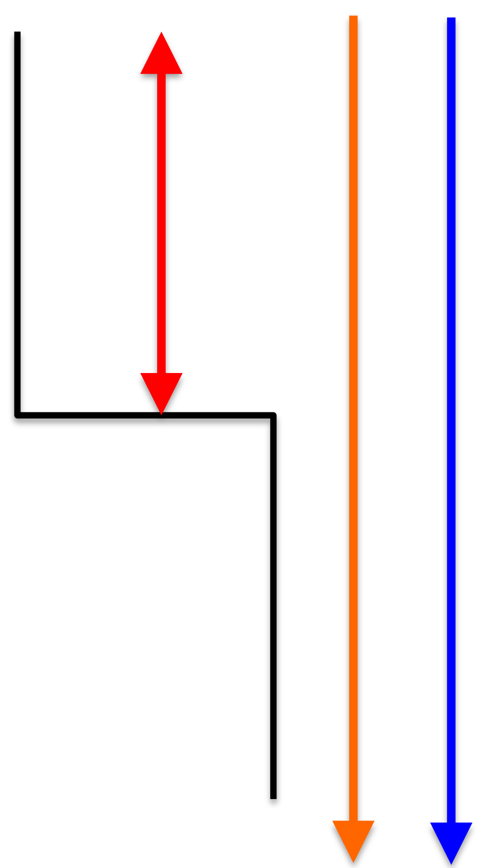
Optical Analogy



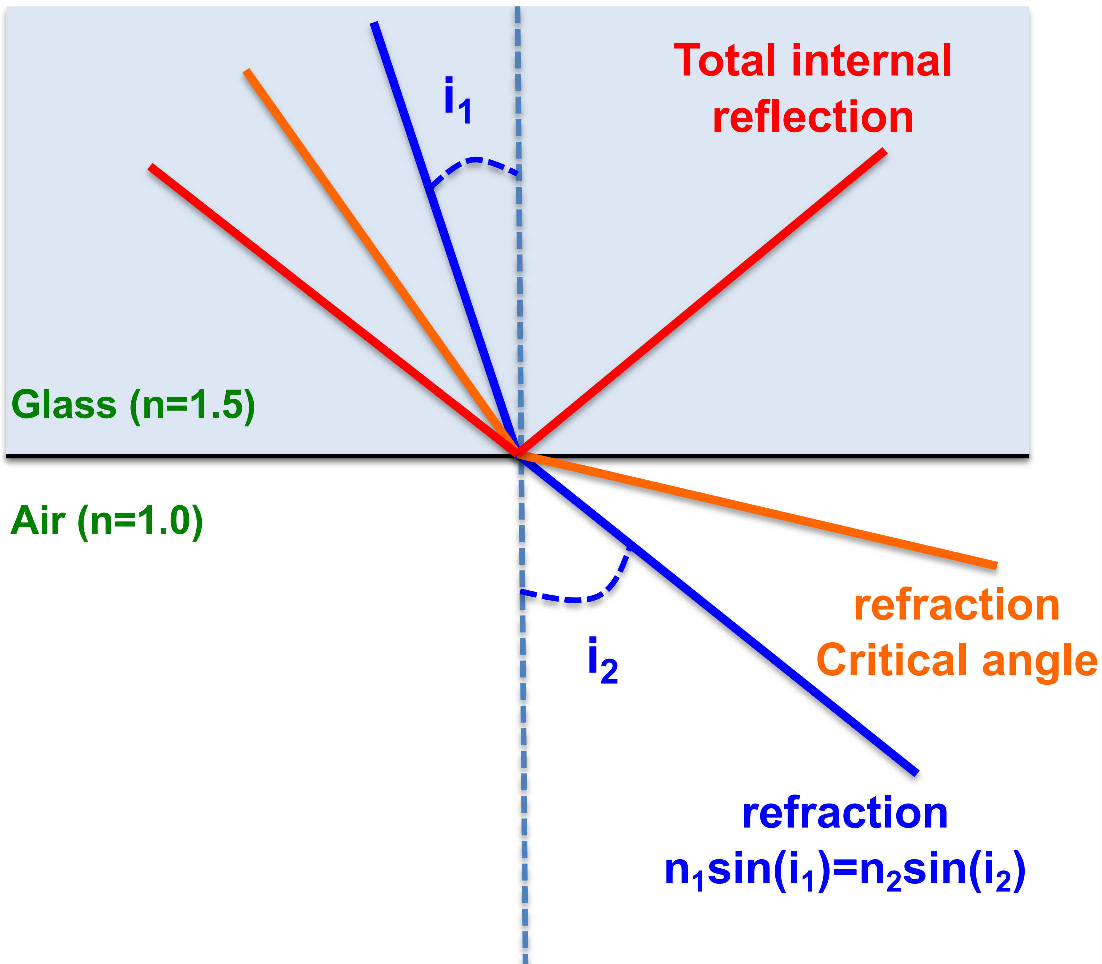
Frustrated total internal reflection

The tunneling effect can be simply observed in wave optics!

Potential barrier



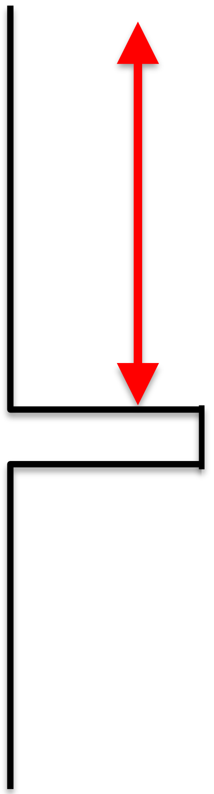
Optical Analogy



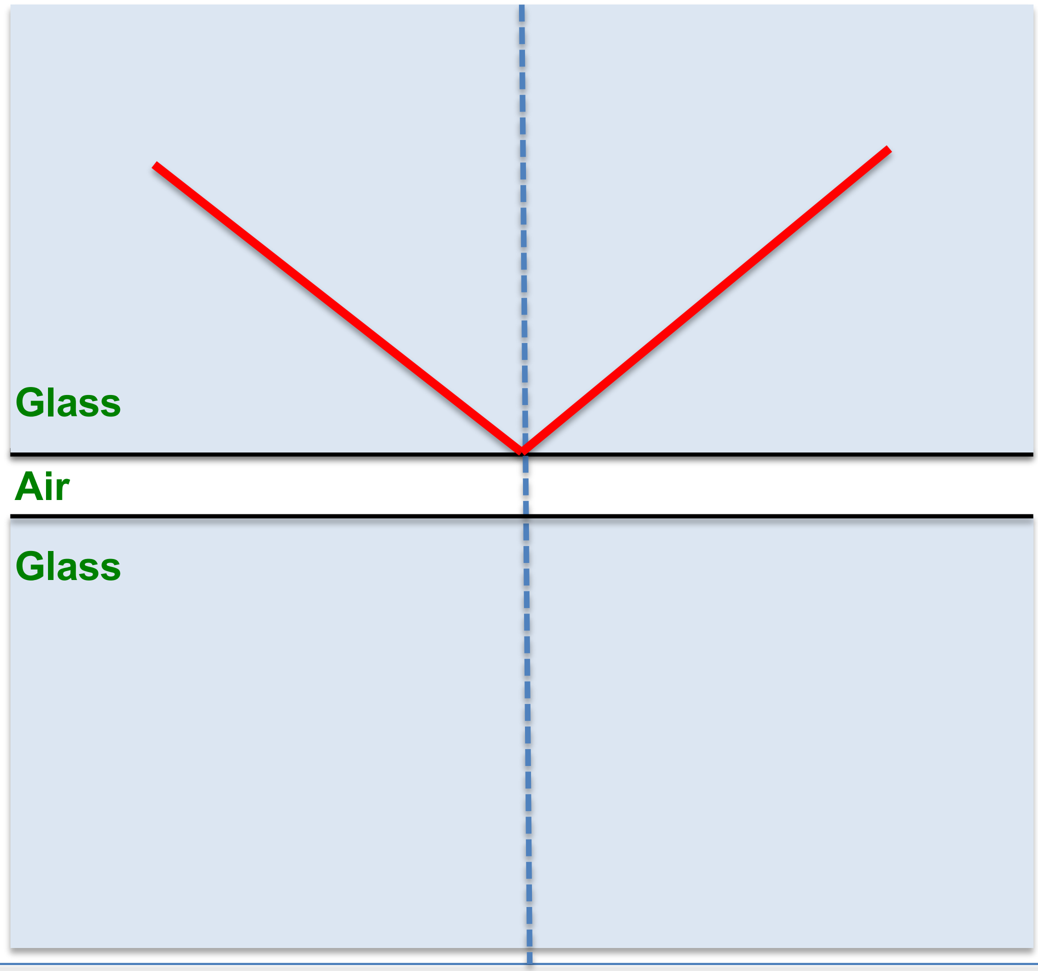
Frustrated total internal reflection

The tunneling effect can be simply observed in wave optics!

Tunnel barrier



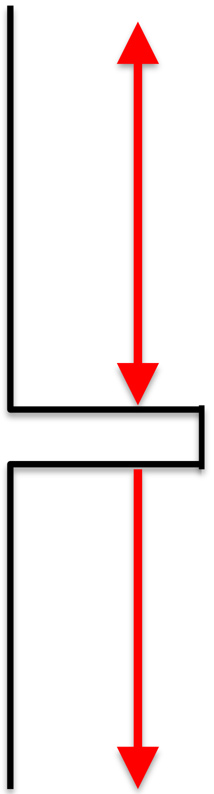
Optical Analogy



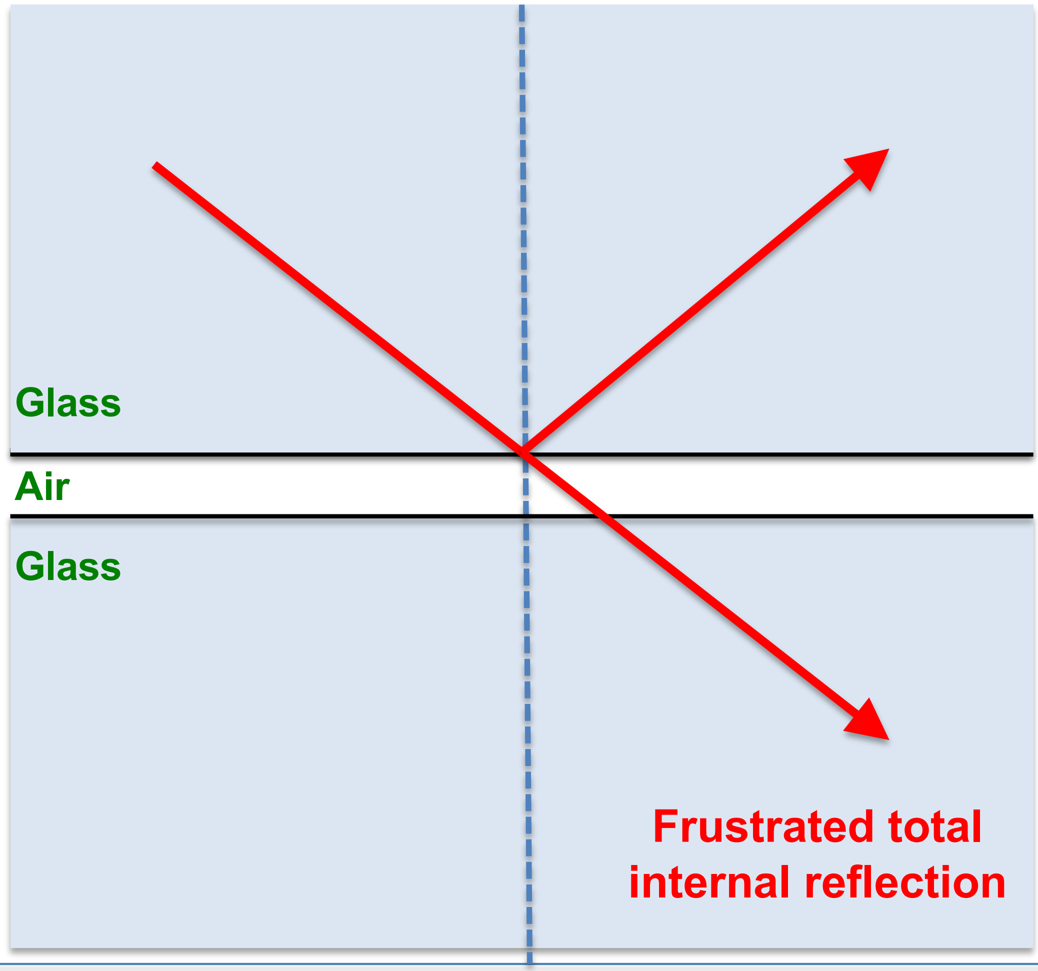
Frustrated total internal reflection

The tunneling effect can be simply observed in wave optics!

Tunnel barrier



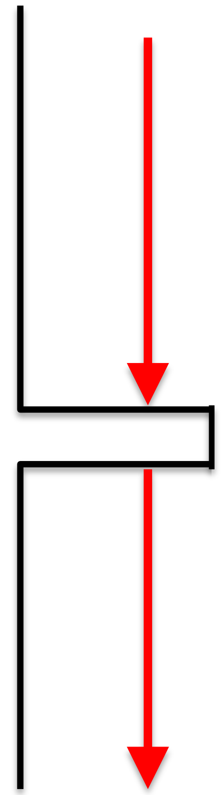
Optical Analogy



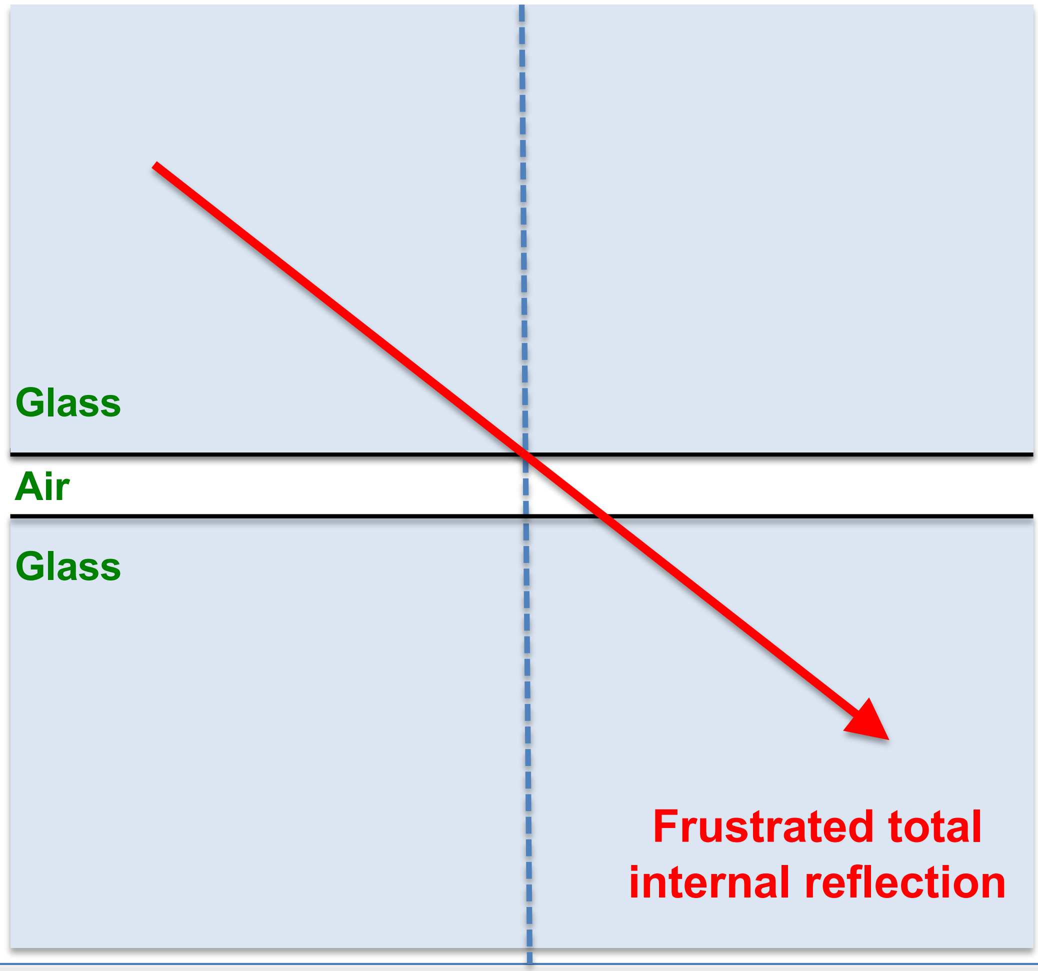
Frustrated total internal reflection

The tunneling effect can be simply observed in wave optics!

Tunnel barrier

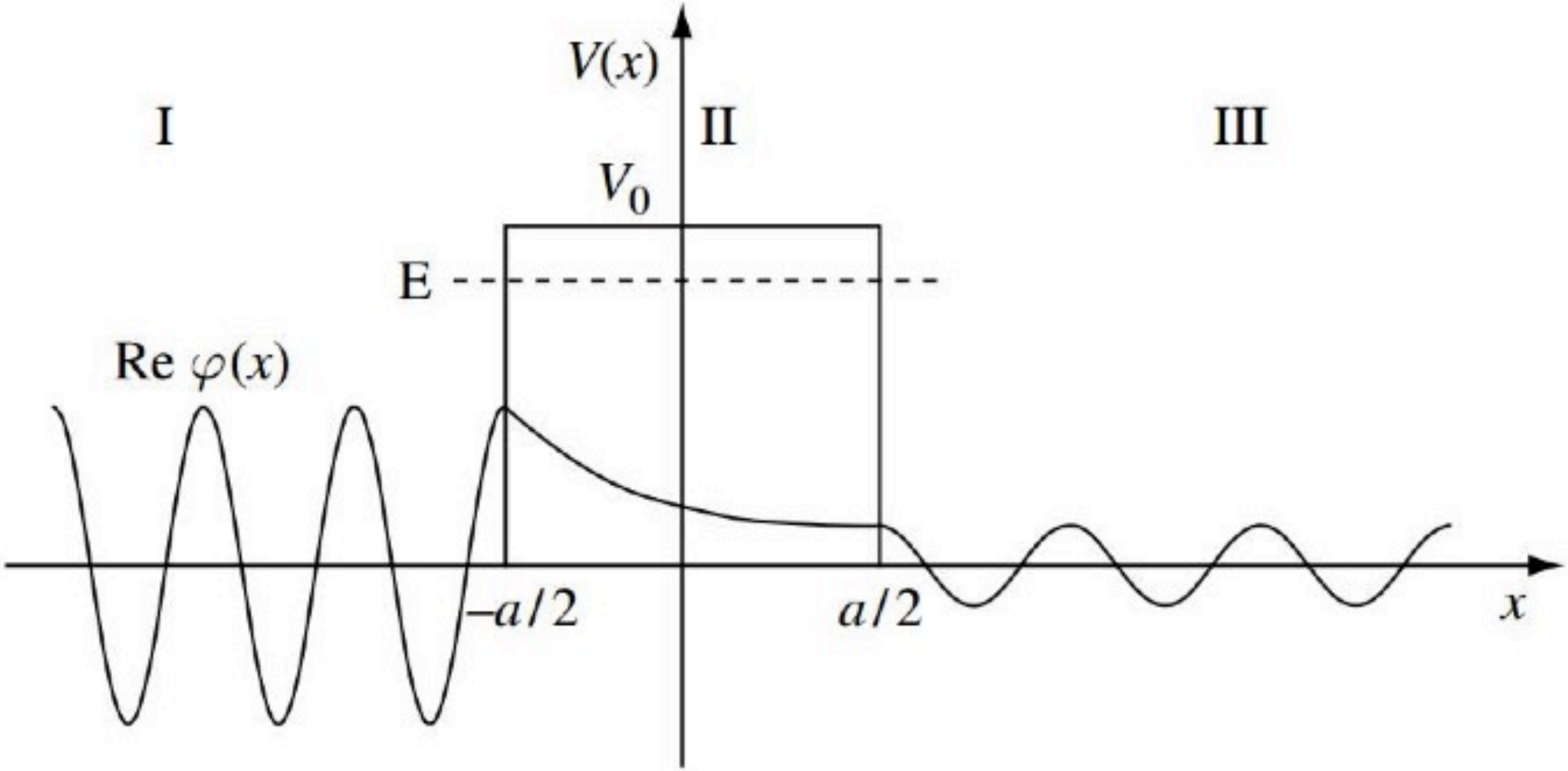


Optical Analogy



Frustrated total internal reflection

Tunelling effect



Similar to an evanescent wave (or a decay wave) in wave optics

Quantum tunneling

Let us give some numbers

$$T = exp(-2a\frac{\sqrt{2mc^2(V_0 - E)}}{\hbar c})$$

$$\hbar c = 197 \text{ eV.nm} = 197 \text{ MeV.fm}$$

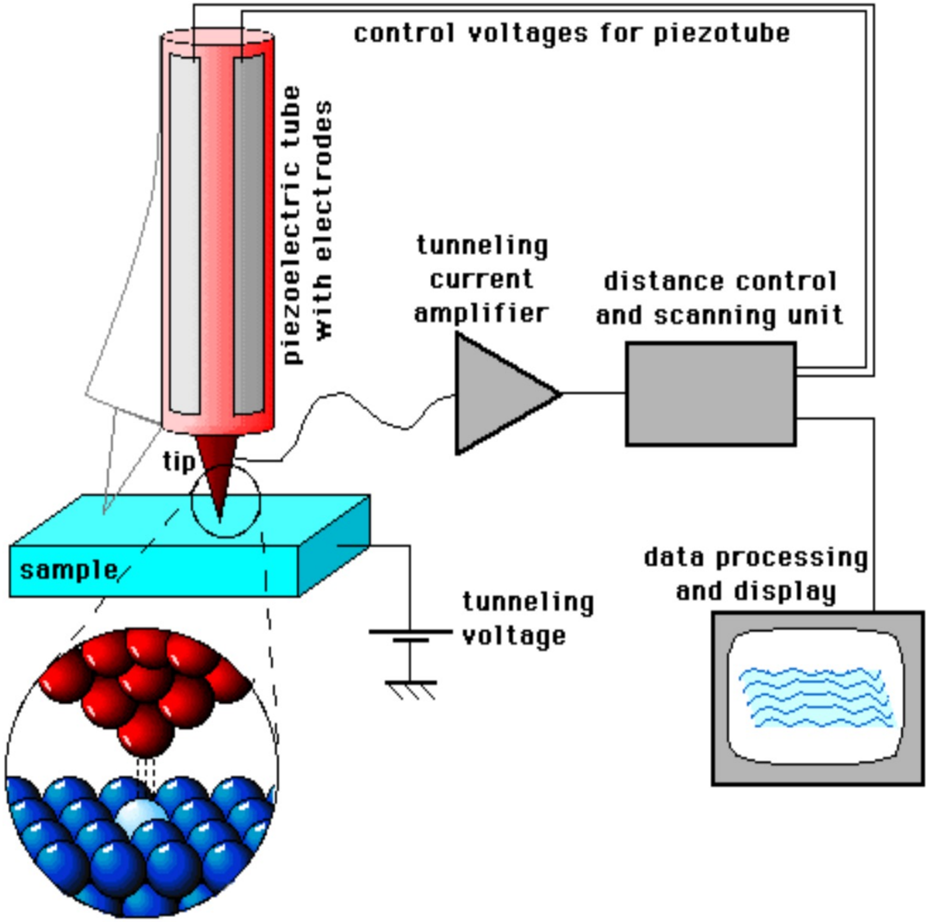
$$a\sqrt{mc^2(V_0 - E)} \sim 100 \text{ eV.nm} \rightarrow T \sim 0.24$$

Consider a transmission coefficient of 0.24

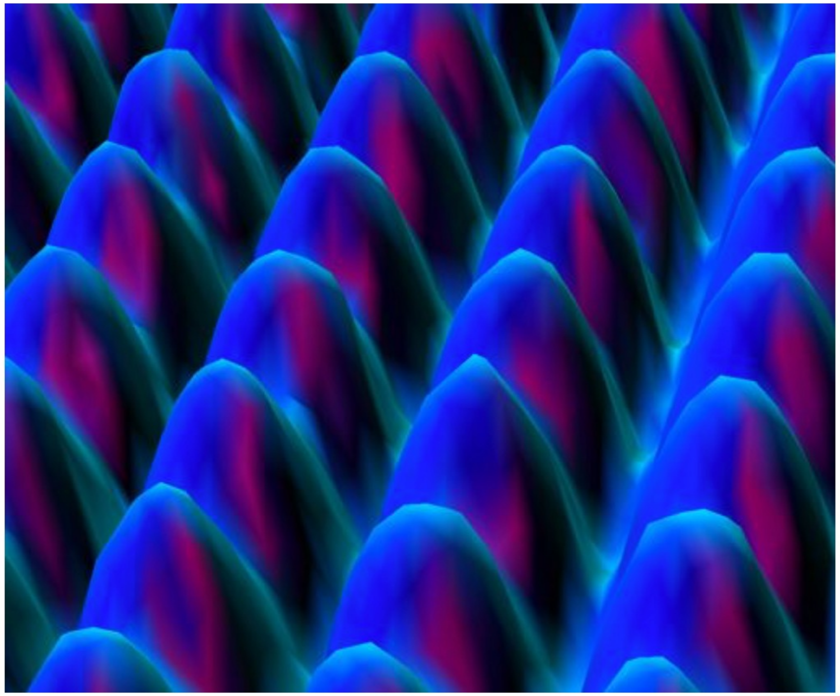
$mc^2 = 100$ GeV $(V_0 - E) = 10$ peV $a = 0.1\ \mu$m	$mc^2 = 1$ GeV $(V_0 - E) = 10$ MeV $a = 1$ fm	$mc^2 = 1$ MeV $(V_0 - E) = 1$ eV $a = 0.1$ nm
Cold atoms	**Nuclear physics**	**Atomic physics**

Universality of the quantum tunneling effect!

Scanning tunneling microscopy



Binning & Rohrer (IBM) 1981-85
Nobel prize winners 1986



Nickel surface, (D. Eigler, IBM)

Electron : V_0-E = 1 eV, a = 5 Angströms : $T \sim 6 \times 10^{-3}$

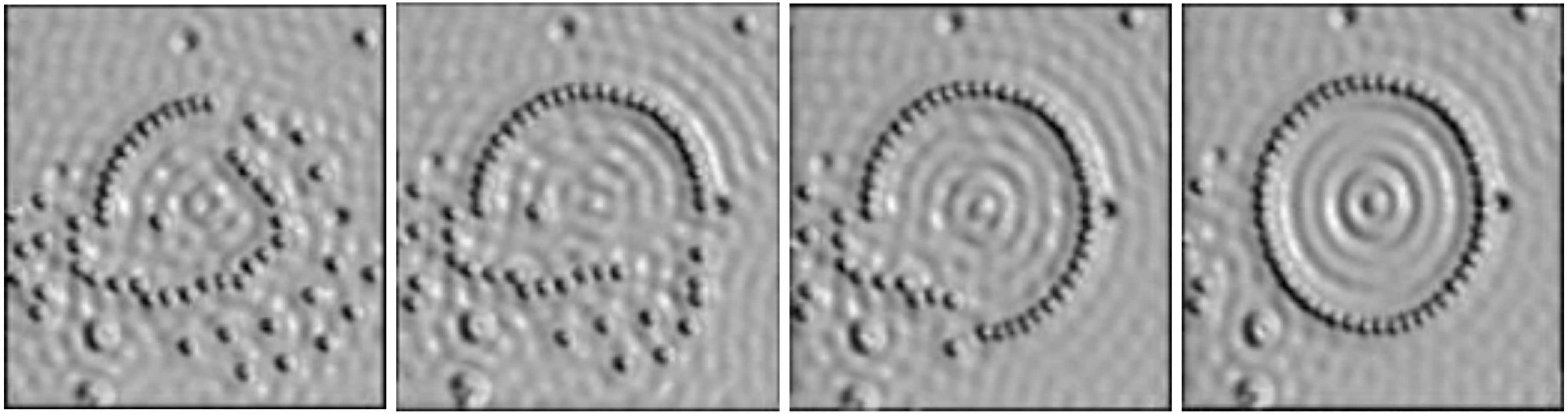
a = 6 Angströms : $T \sim 2 \times 10^{-3}$

The tunneling current changes very quickly with the distance (due to the exponential term in the transmission coefficient)

Scanning tunneling microscopy

Moving atoms one by one

Nanomanipulation: The STM tip is used to lift and put down the atomic units

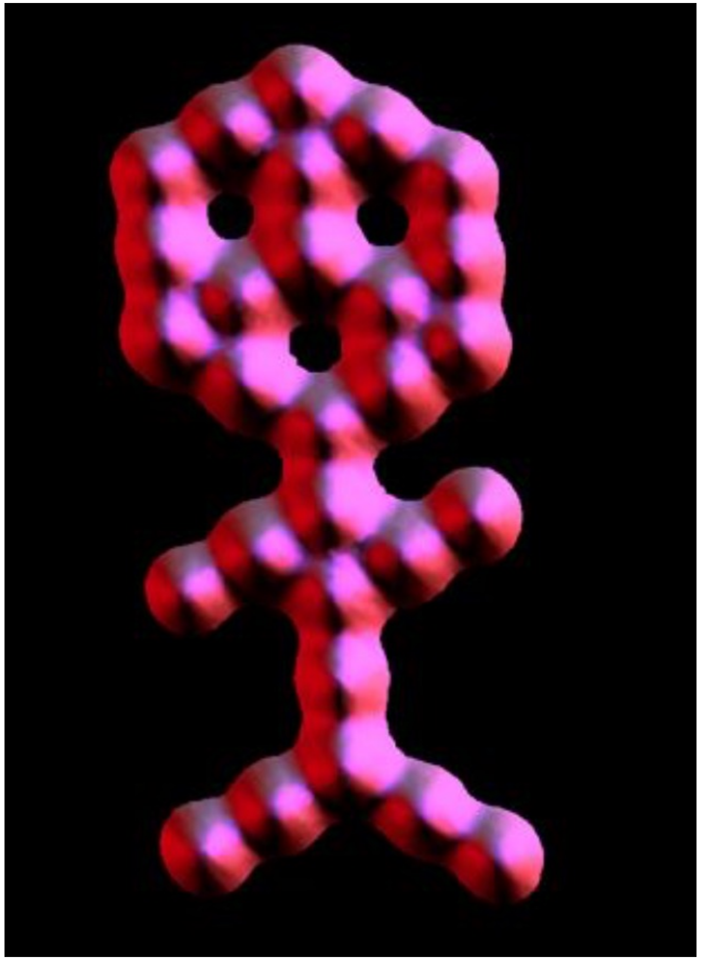


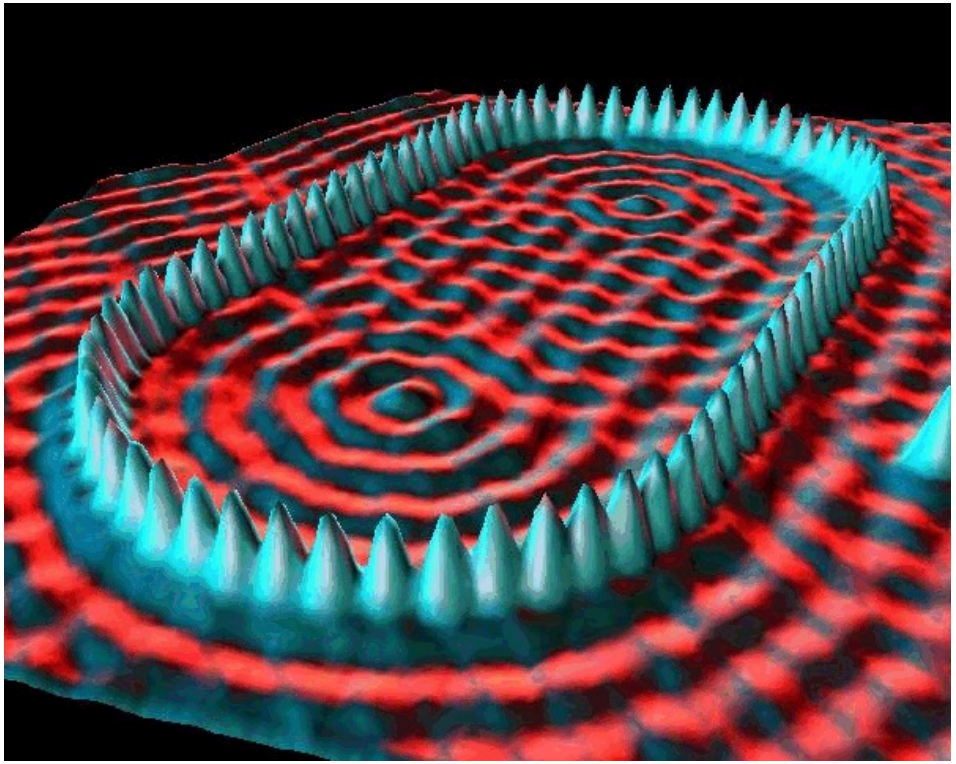
1 **2** **3** **4**

A set of STM images showing formation of a quantum coral from 48 Fe atoms adsorbed on the surface of Cu(111)

Moving atoms one by one

Carbon monoxide man (IBM)

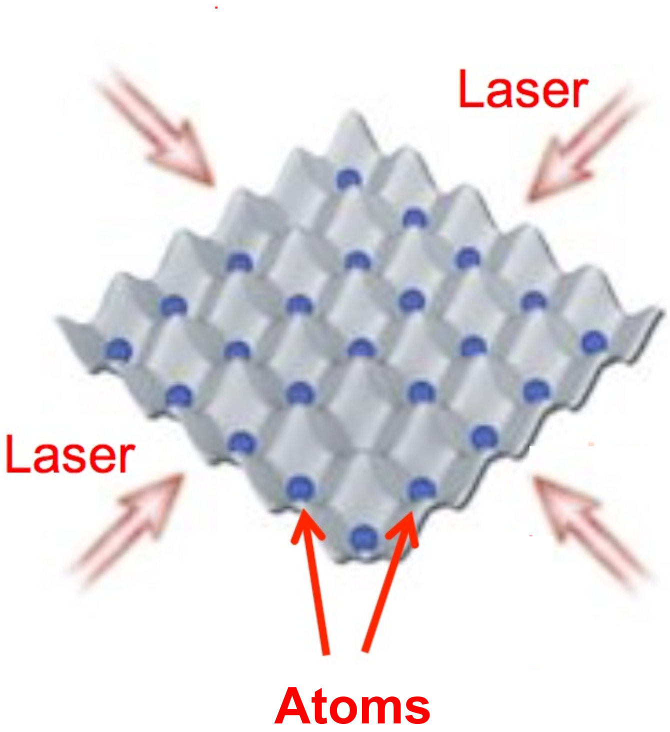


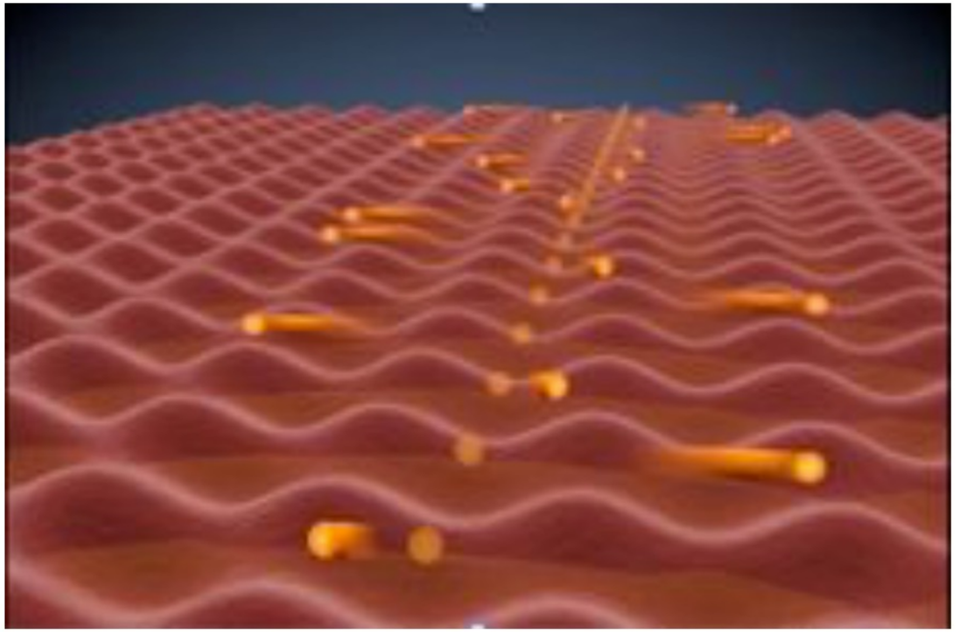


Stadium coral: Iron atoms on a copper surface (IBM)

Ultracold atoms

We use set of lasers to localize atoms (standing wave)



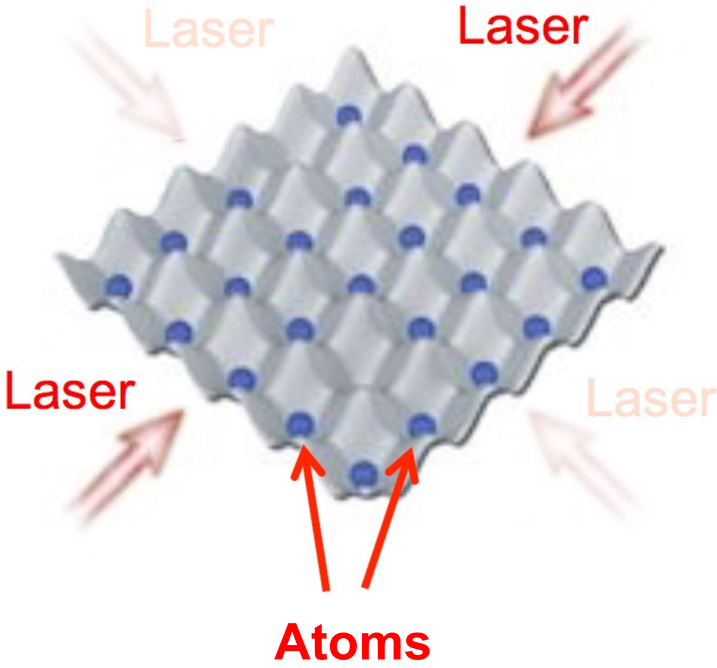


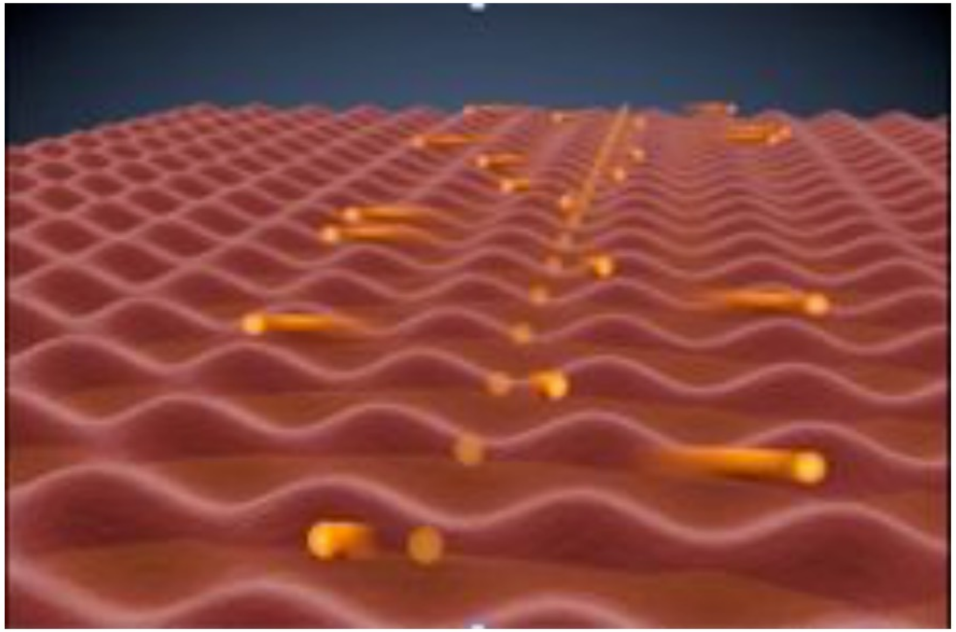
v= 5 mm/s, 100 nK
10 peV, λ_{dB}=1 micron

The lattice potential is reduced and then we let atoms tunnel for a given time and finally we can measure their positions (wave packet spreading → time of flight measurement)

Ultracold atoms

We use set of lasers to localize atoms (standing wave)

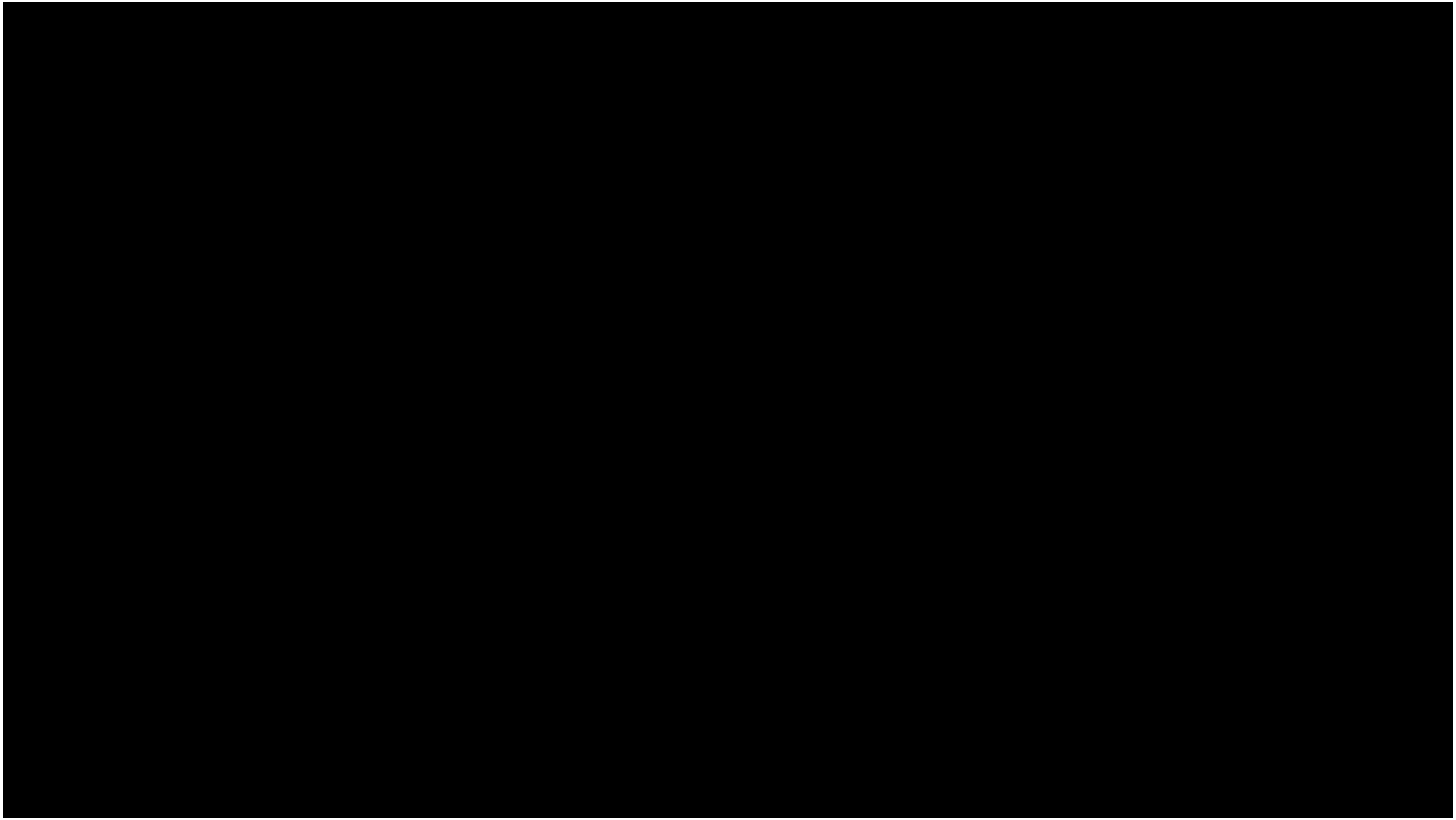




v= 5 mm/s, 100 nK
10 peV, λ_{dB}=1 micron

The lattice potential is reduced and then we let atoms tunnel for a given time and finally we can measure their positions (wave packet spreading → time of flight measurement)

Quantum horse race



C. Weitenber et al., Nature, vol. 471, pp. 319, (2011)

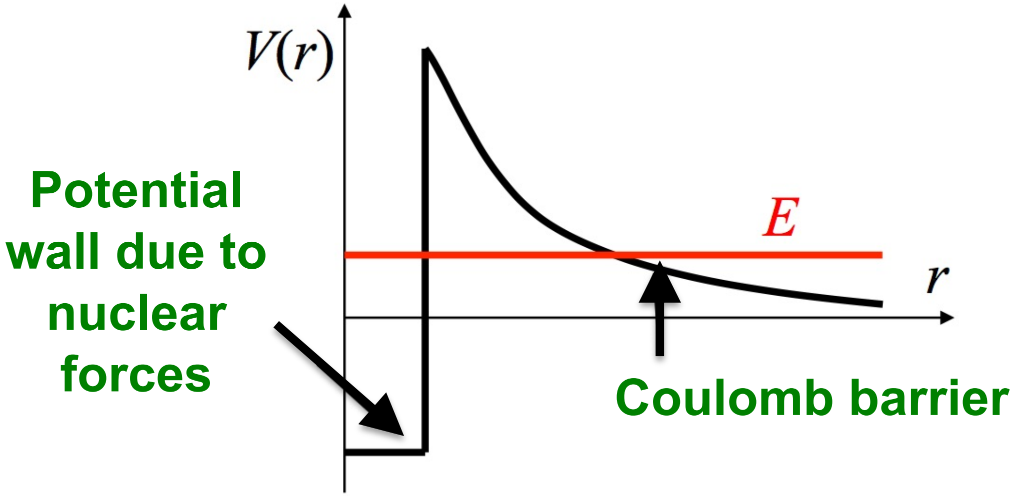
Alpha radioactive decay

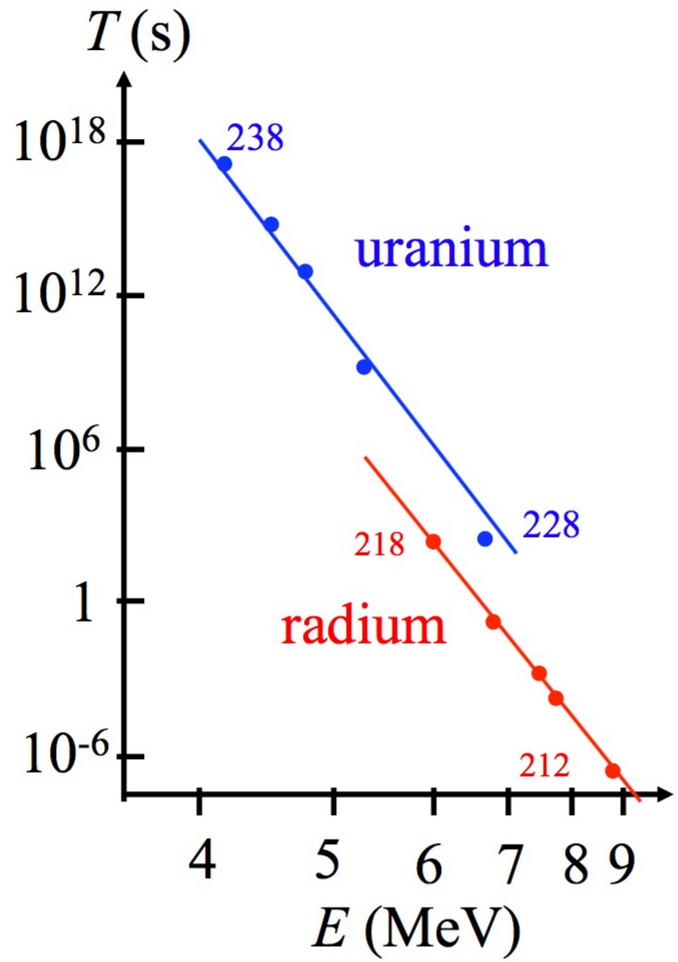
Alpha decay or α-decay is a type of radioactive decay in which an atomic nucleus emits an alpha particle (helium nucleus)

$$^{A}_{Z}X \quad \rightarrow \quad ^{A-4}_{Z-2}Y \ + \ ^{4}_{2}\mathrm{He}$$

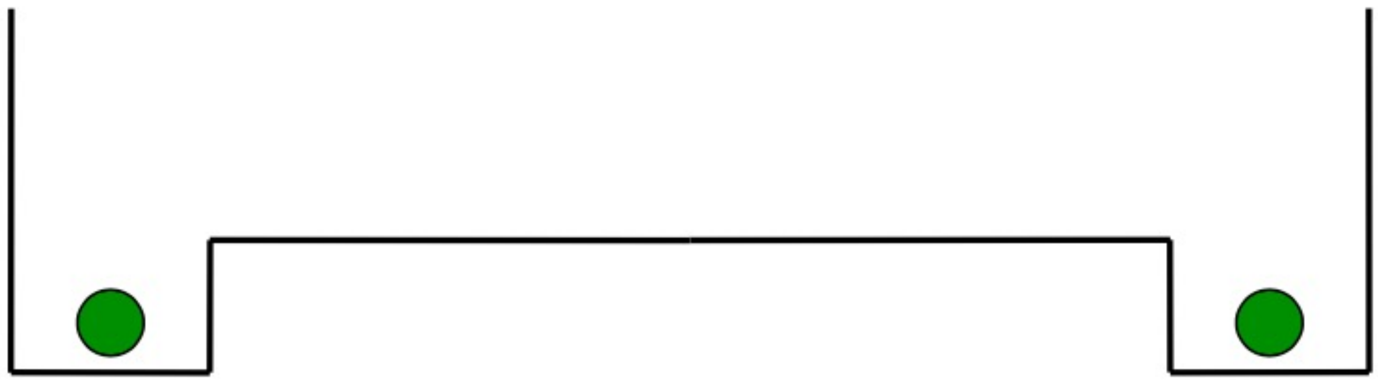
Energy of the particle E is 4 to 9 MeV
Probability of disintegration T is 10^{-6} s to 10^{18} s

Gamow 1929 : $$\log T = a + \frac{b}{\sqrt{E}}$$



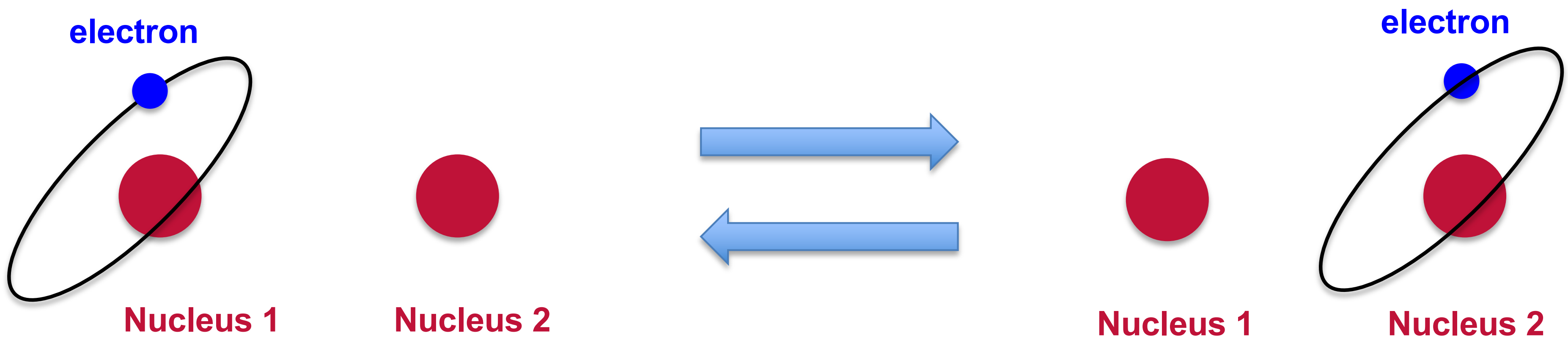


4.
Double well potential



How to explain the chemical bond?

2 nuclei and 1 electron (Dihydrogen cation i.e. ion H_2^+)

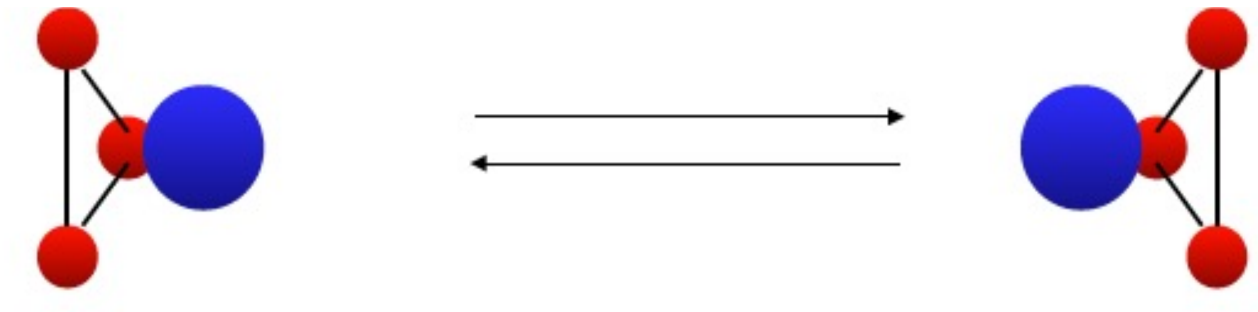


We will show that the tunneling jump of the electron from orbit 1 to orbit 2 lowers the energy. This effect is enhanced when the two nuclei are located relatively close to each other

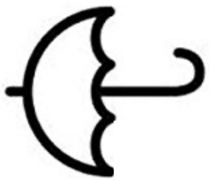
Attraction between atoms explains the chemical bond

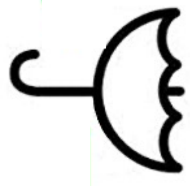
Ammonia (NH_3)

Under the right conditions, ammonia molecules can be flipped. Imagine you are looking at an open umbrella from the side. A strong wind comes along and turns the umbrella inside out!



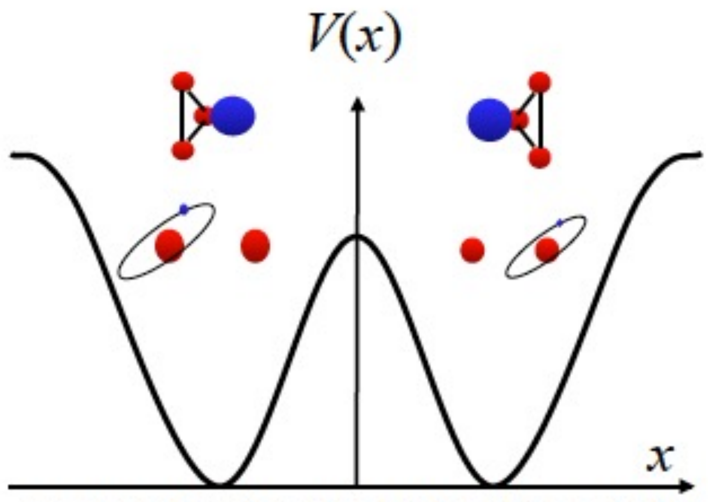
Left configuration **Right configuration**

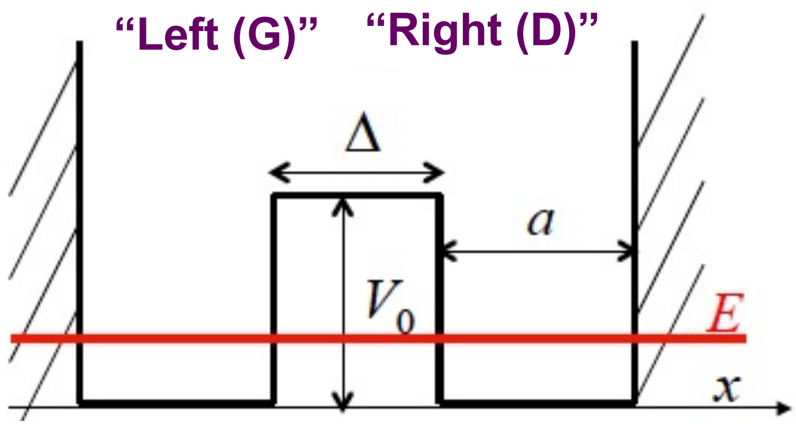




The fundamental state of the molecule is in a superposition of two configurations « Left » and « Right », hence quantum oscillations take place between the two states through tunneling effect

Double well potential





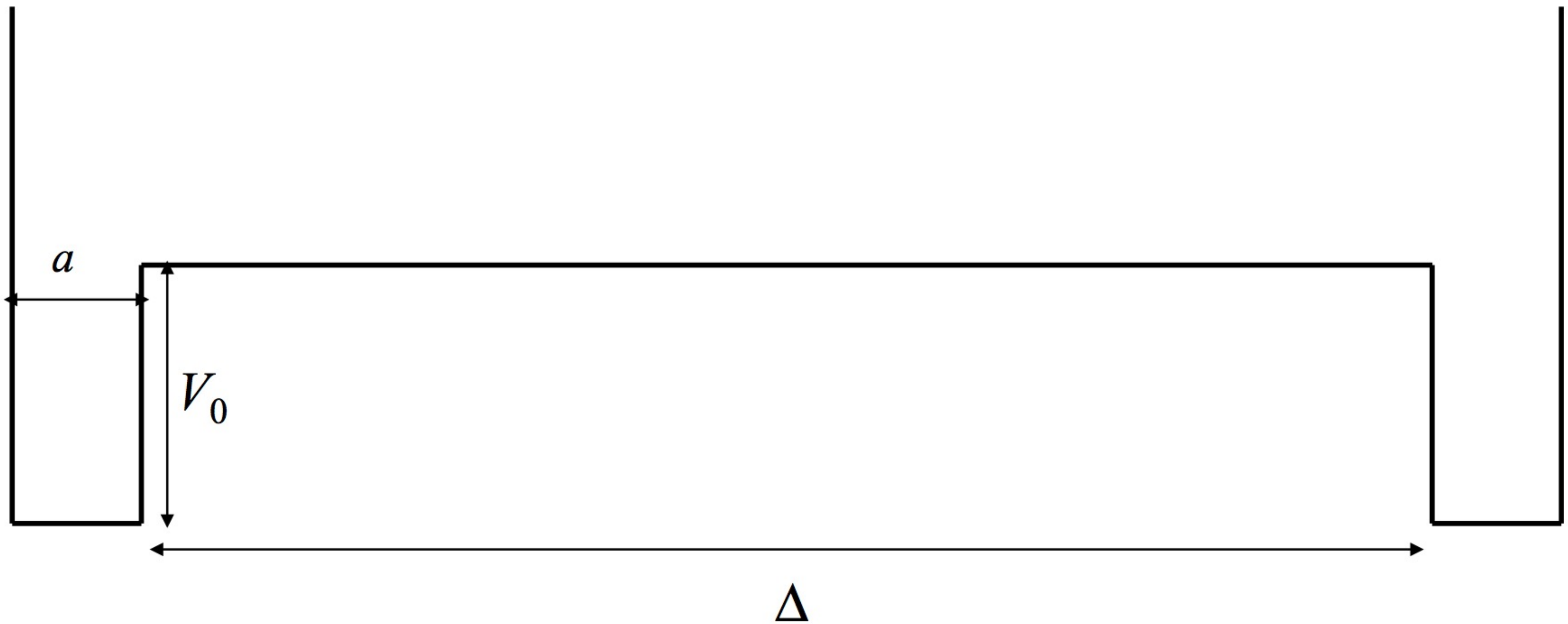
Consider the energy levels such as $E<V_0$

What is the role of the tunneling effect across the barrier ?

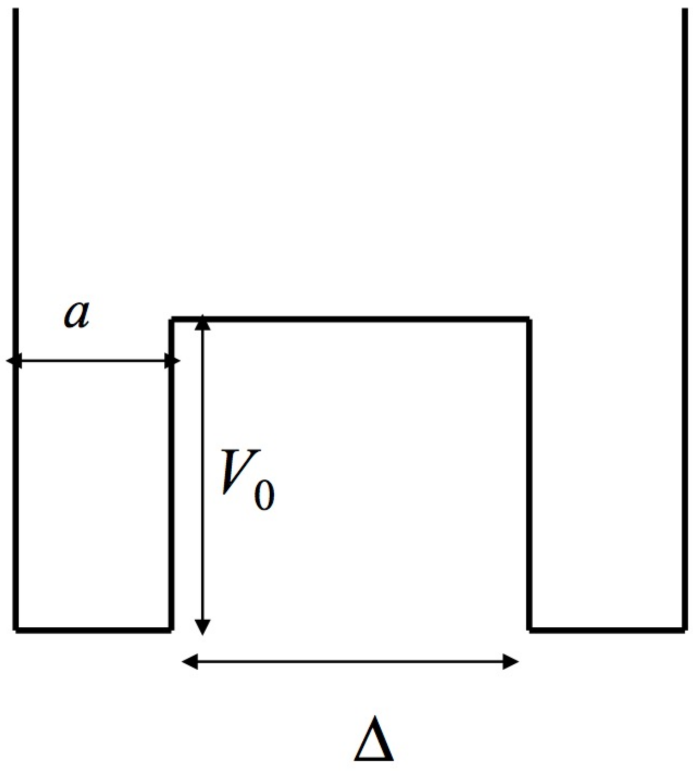
As the Hamiltonian H(x) is invariant i.e. H(-x) = H(x), the eigenstates of the Hamiltonian can be described through a linear combination of even (symmetric) and odd (antisymmetric) functions

$$\psi(x) = \psi(-x) \qquad \psi(x) = -\psi(-x)$$

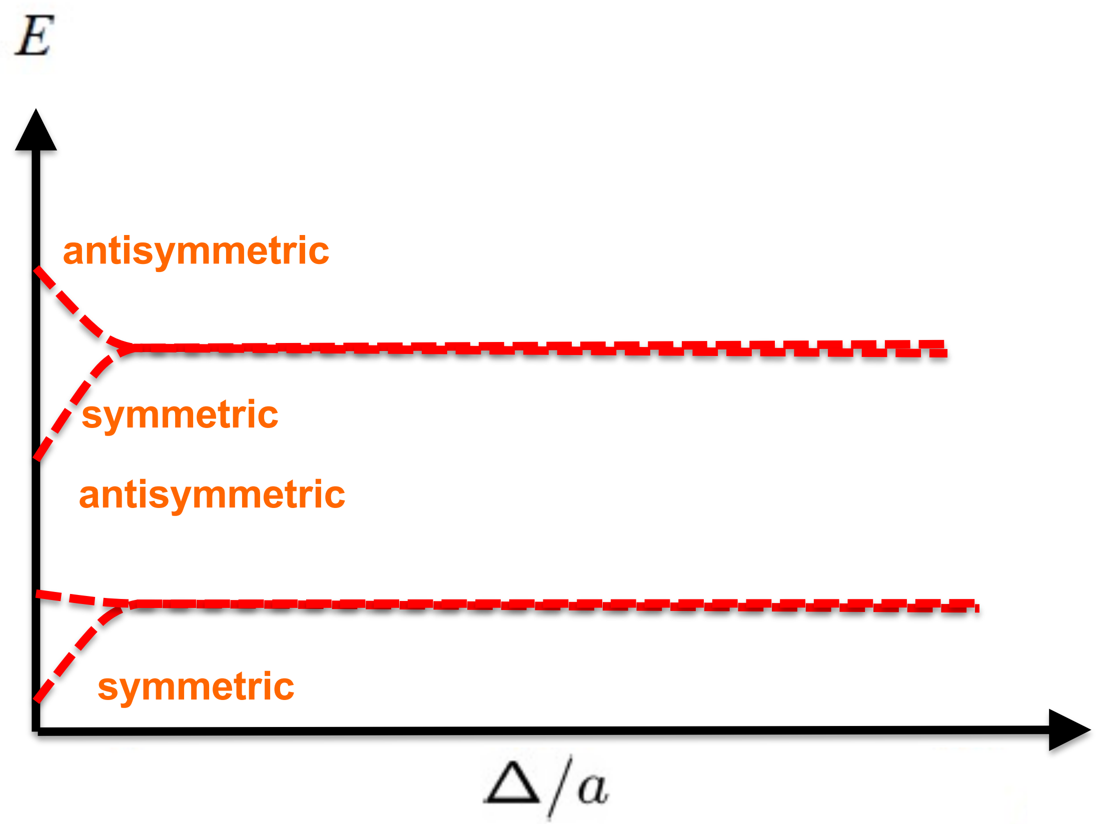
Double well potential



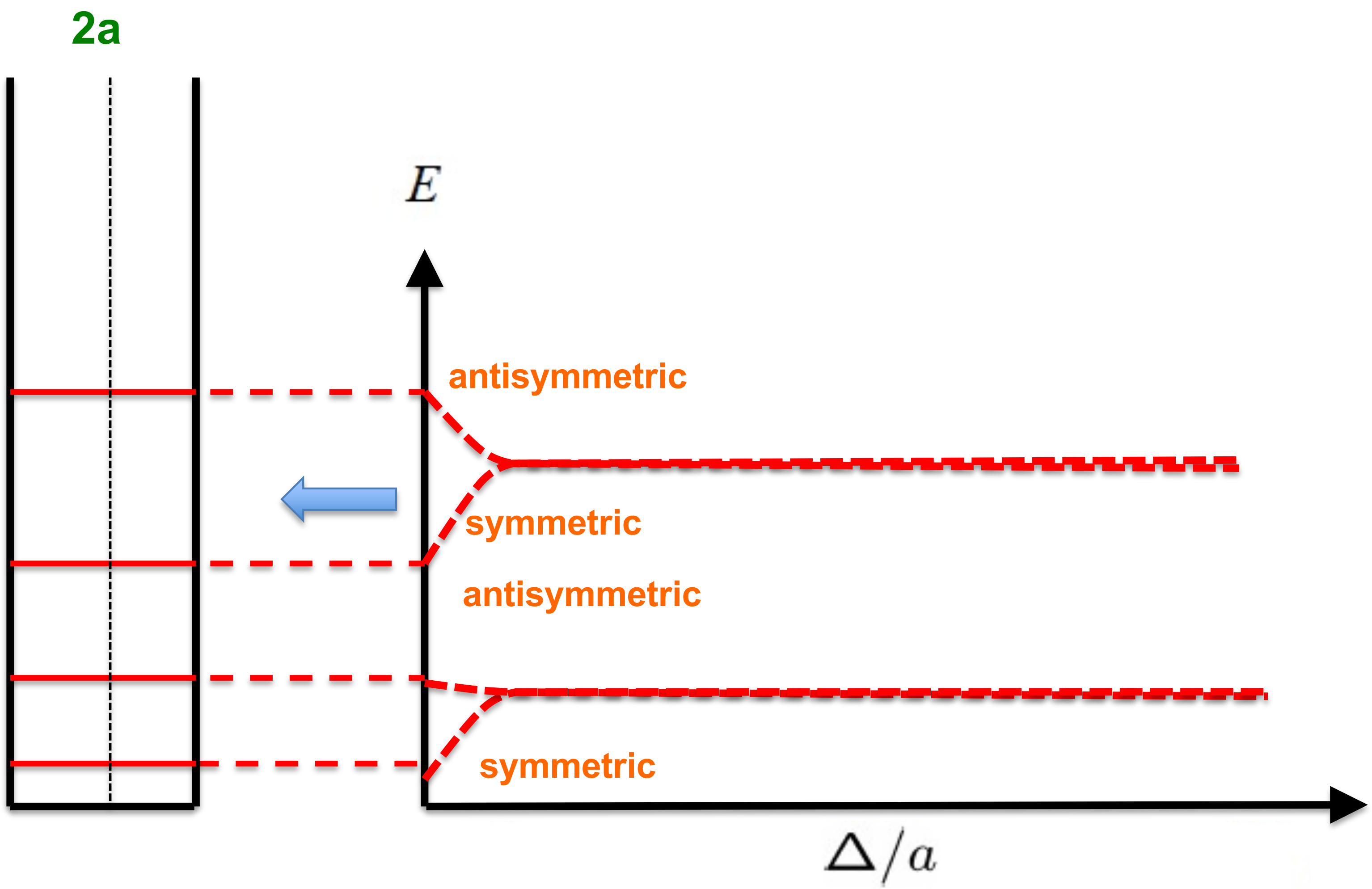
Double well potential



Energy levels

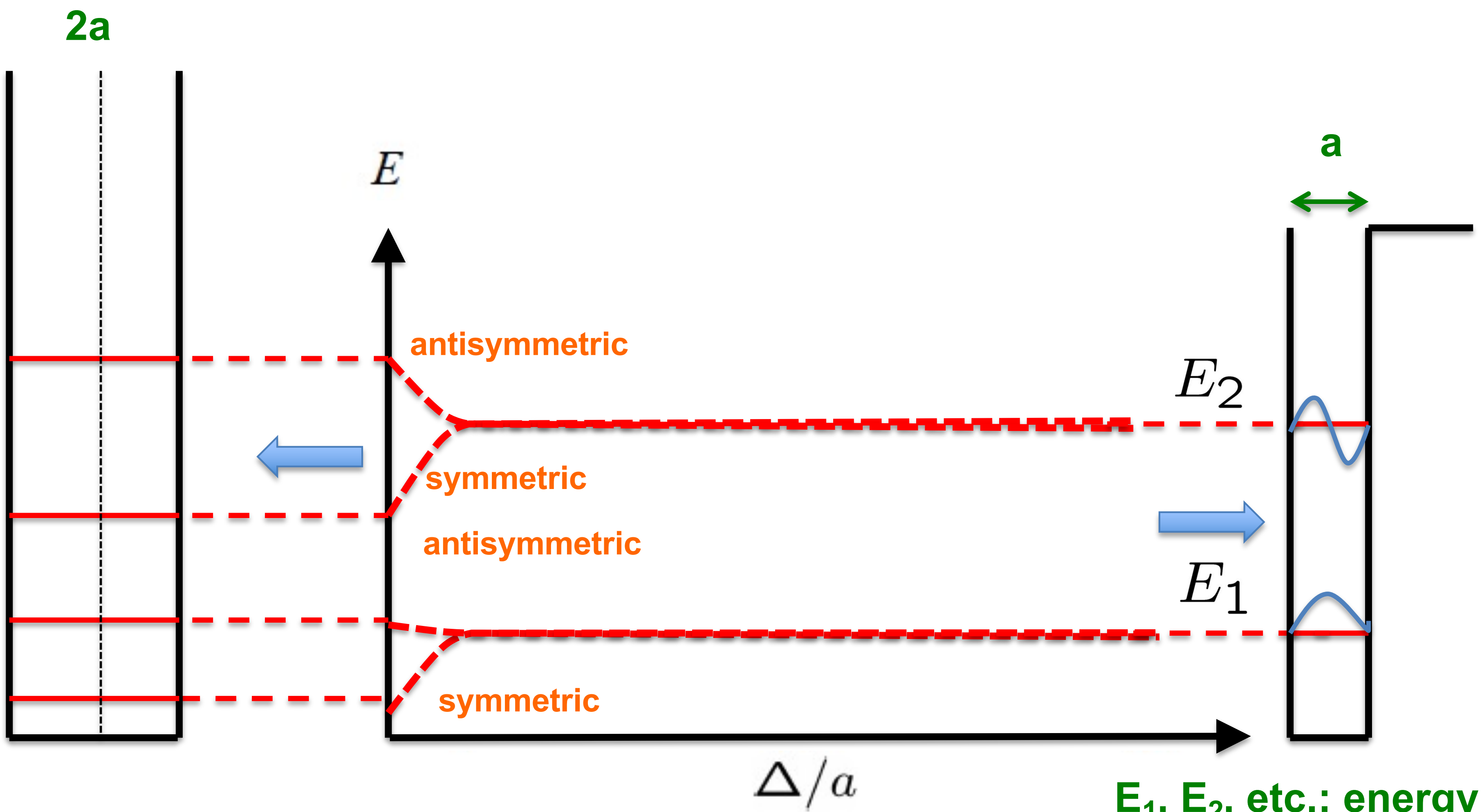


Energy levels



Infinite well
Width 2a

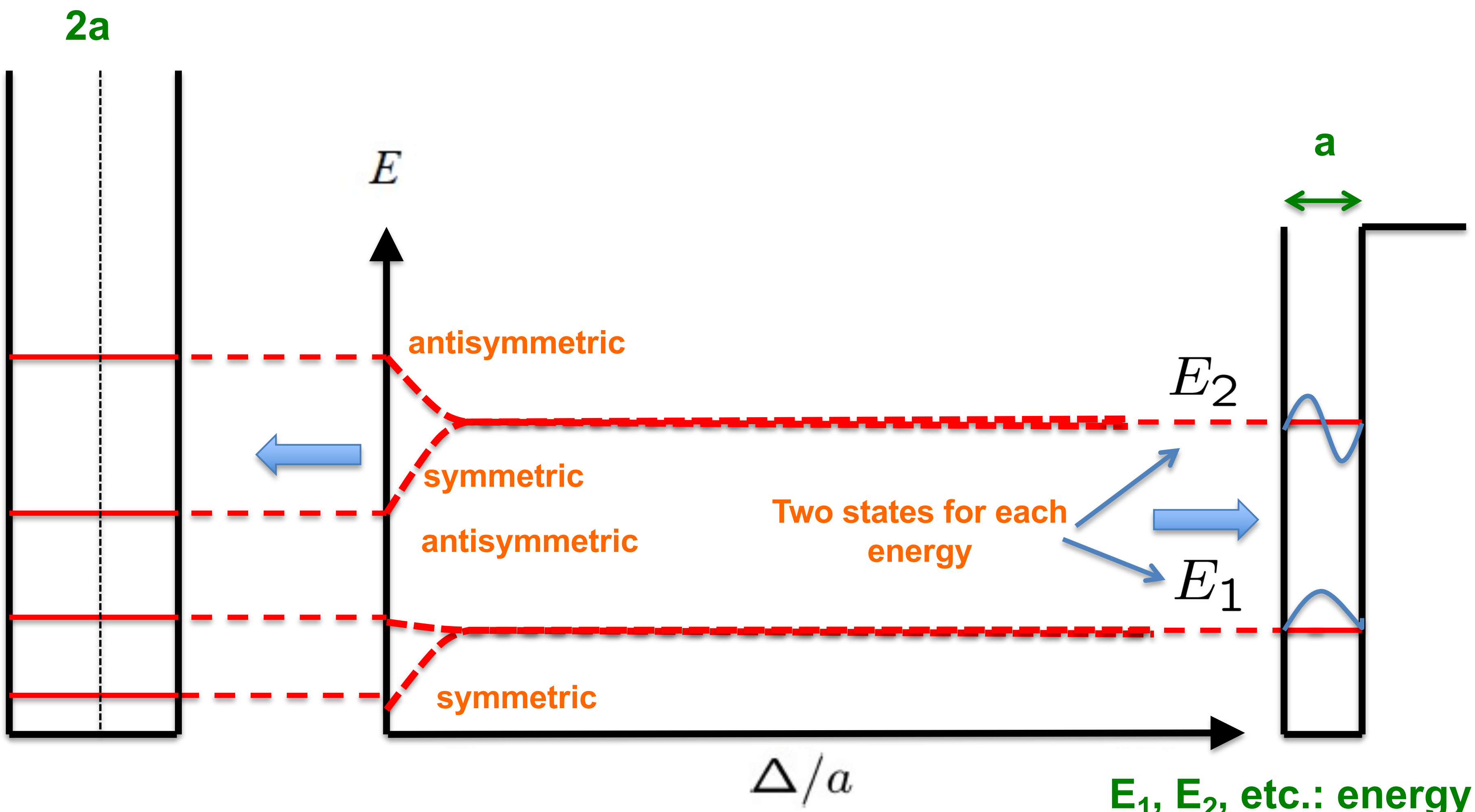
Energy levels



Infinite well
Width 2a

E_1, E_2, etc.: energy levels of semi-infinite well of width a

Energy levels

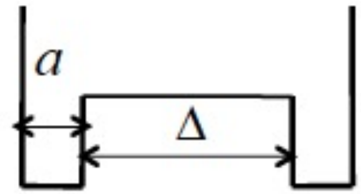


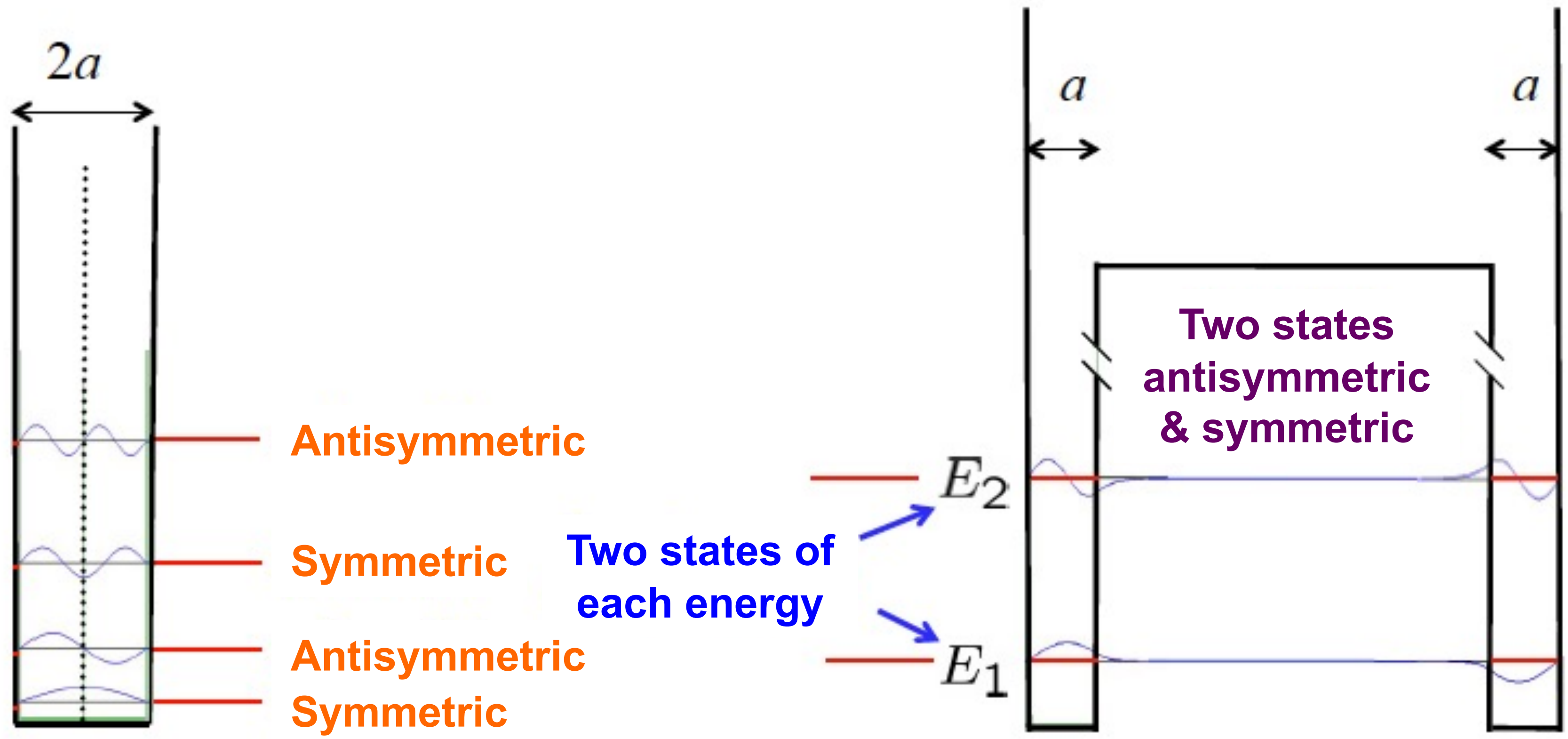
Infinite well
Width 2a

E_1, E_2, etc.: energy levels of semi-infinite well of width a

The tunneling effect raises the degeneracy of the two initial states

Energy levels

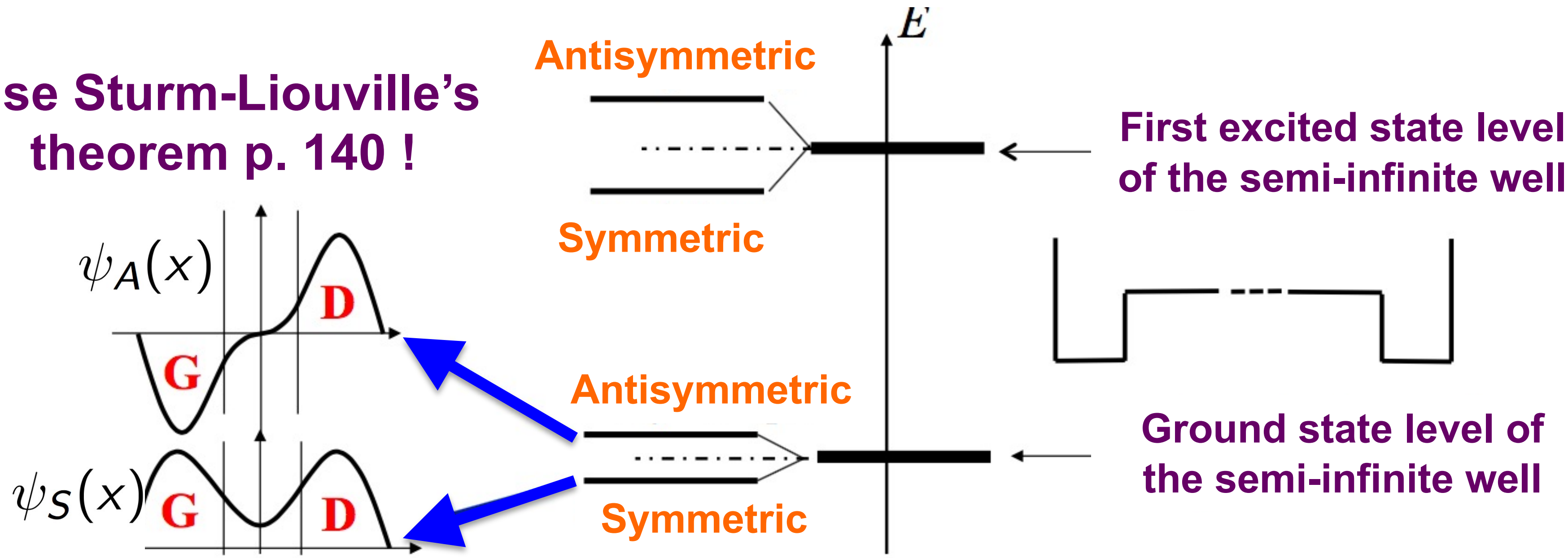




The molecule appears in a superposition of two configurations « Left » and « Right », with quantum oscillations taking place between the two states through tunneling effect

Summary

Use Sturm-Liouville's theorem p. 140 !



$$E_A = E_1 + A$$

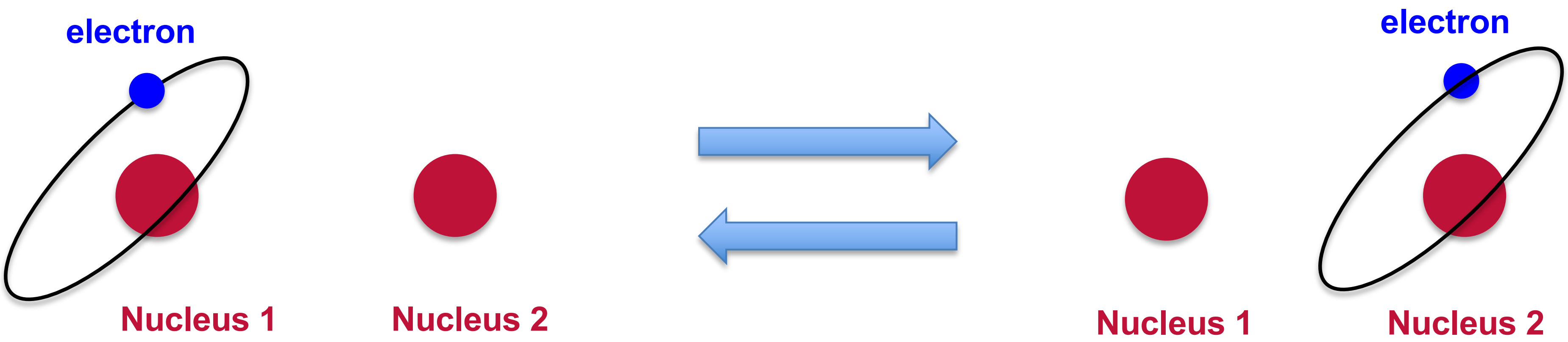
$$E_S = E_1 - A$$

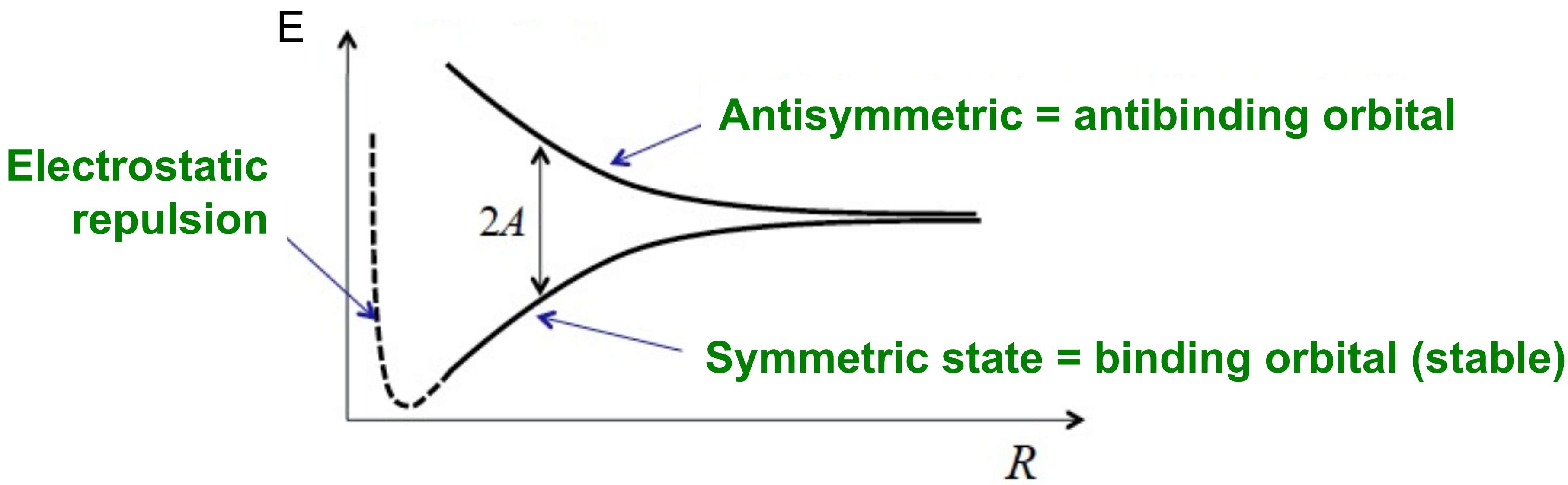
with $$A = \frac{2\hbar^2\pi^2}{m\kappa a^3}\, e^{-\kappa\Delta}$$

if $V_0 \gg E$ $\qquad \kappa \simeq \sqrt{2mV_0}/\hbar \qquad \kappa a\ ,\ \kappa\Delta \gg 1$

Chemical bond

The cleavage 2A depends on the distance R between the two nuclei





Ammonia in an electric field

Objective: Using this molecule as a source of radiation

Operation in two steps

(1) How to transfer energy to the molecule?
Population inversion is obtained by using a static electric field to select a given quantum state

(2) How to extract this energy as a radiation?
Stimulated emission of radiation is obtained by using an oscillating electric field at frequency ω_0

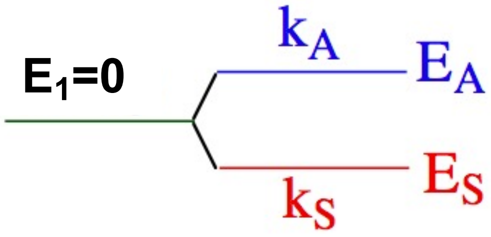
Amplification by stimulated emission of radiation

MASER (small spontaneous emission with microwaves)

LASER (large spontaneous emission with light)

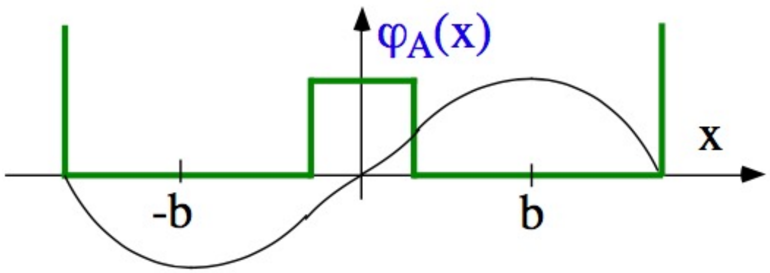
Ammonia inversion

Consider the ammonia inversion doublet with the lowest energy level



$$\Delta E = E_A - E_S = \frac{\hbar^2\pi^2}{2ma^2} \times \frac{8\, e^{-\kappa\,\Delta}}{\kappa\, a}$$

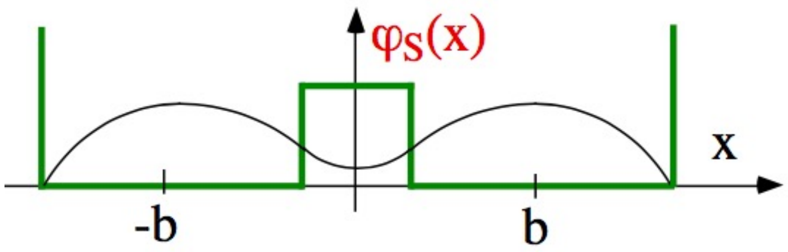
$$E_A - E_S = \hbar\omega_0, \quad E_A + E_S = 0$$



For both eigenstates

$$\psi_{A,S}(x,t) = \varphi_{A,S}(x)e^{-iE_{A,S}\,t/\hbar}$$

$$|\,\psi_{A,S}(x,t)\,|^2 = |\,\varphi_{A,S}(x)\,|^2$$



Probability densities are symmetric and time independent (i.e. stationary states) with values of ½ for each state

Ammonia inversion

$$\hat{A} = \begin{pmatrix} a & b+ic \\ b-ic & d \end{pmatrix}$$

general expression with
a, b, c, and d real numbers

The Hamiltonian in the basis is $(|\varphi_A\rangle, |\varphi_S\rangle)$ diagonal

$(|\varphi_A\rangle, |\varphi_S\rangle)$ are eigenstates of the $\hat{H}_{NH_3}$

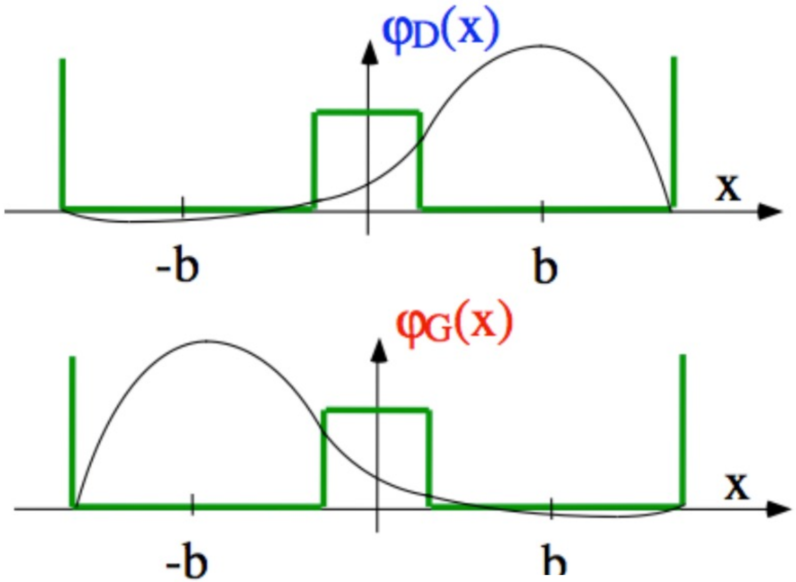
with eigenvalues
$$E_A = E_1 + A = \frac{\hbar\omega_0}{2}$$

(Taking E_1=0)

$$E_S = E_1 - A = -\frac{\hbar\omega_0}{2}$$

then
$$\hat{H}_{NH_3} = \begin{pmatrix} E_A & 0 \\ 0 & E_S \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

Ammonia inversion



Consider the quantum superpositions

$$|\varphi_D\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_S\rangle + |\varphi_A\rangle\right)$$ **"Right (D)"**

$$|\varphi_G\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_S\rangle - |\varphi_A\rangle\right)$$ **"Left (G)"**

Those are not stationary states!

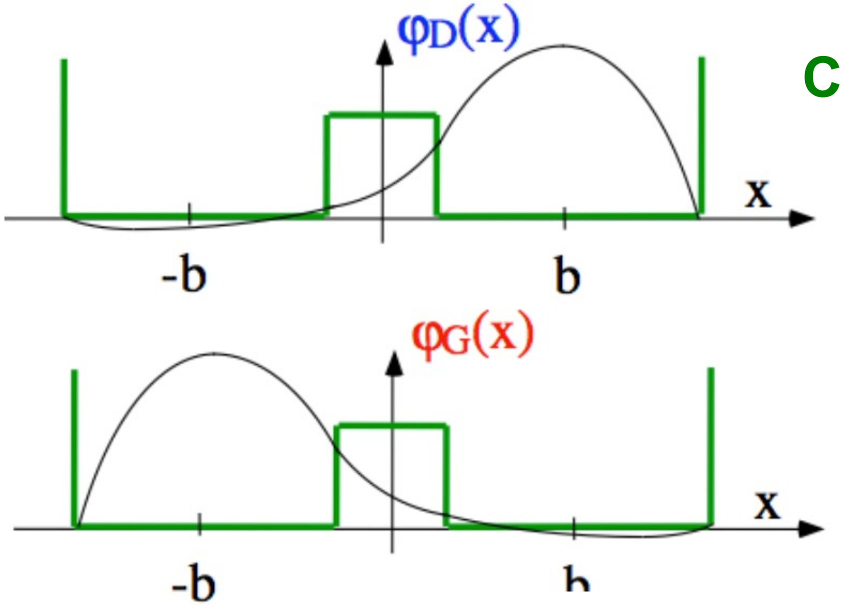
If $$|\psi(t=0)\rangle = |\varphi_D\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_S\rangle + |\varphi_A\rangle\right)$$

then $$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_S t/\hbar}|\varphi_S\rangle + e^{-iE_A t/\hbar}|\varphi_A\rangle\right)$$

$$|\psi(t)\rangle = \frac{1}{2}\left[\left(|\varphi_D\rangle + |\varphi_G\rangle\right)e^{i\omega_0 t/2} + \left(|\varphi_D\rangle - |\varphi_G\rangle\right)e^{-i\omega_0 t/2}\right]$$

$$|\psi(t)\rangle = \cos\left(\frac{\omega_0 t}{2}\right)|\varphi_D\rangle + i\sin\left(\frac{\omega_0 t}{2}\right)|\varphi_G\rangle$$

Ammonia inversion



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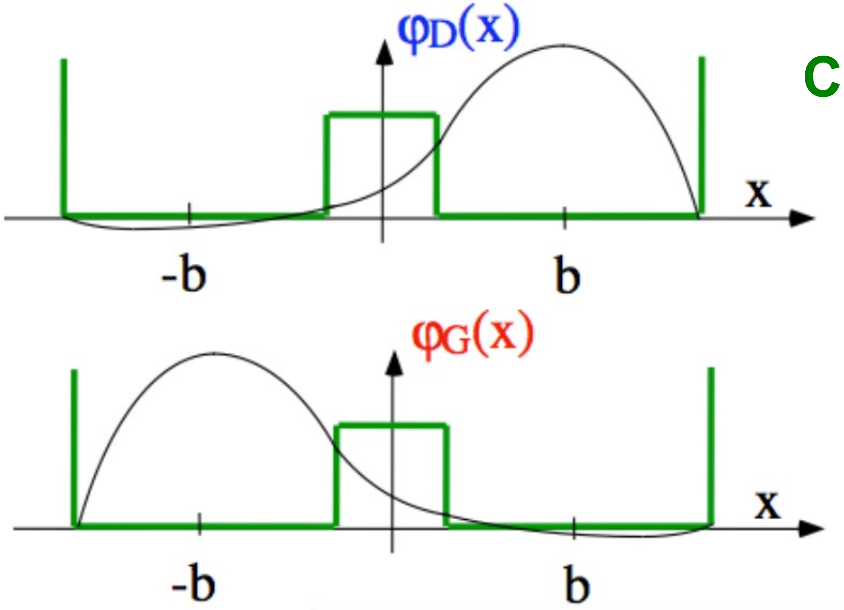
$$|\varphi_G\rangle = \frac{1}{\sqrt{2}}(|\varphi_S\rangle - |\varphi_A\rangle)$$ **"Left (G)"**

If $$|\psi(t)\rangle = \cos\left(\frac{\omega_0 t}{2}\right)|\varphi_D\rangle + i\sin\left(\frac{\omega_0 t}{2}\right)|\varphi_G\rangle$$

If the molecule is initially prepared to be in the "Right" configuration, over time, the molecule will be oscillating at frequency ω_0 between "Right" and "Left" dispositions

Nitrogen inversion → oscillating dipole → radiation at frequency

Ammonia inversion



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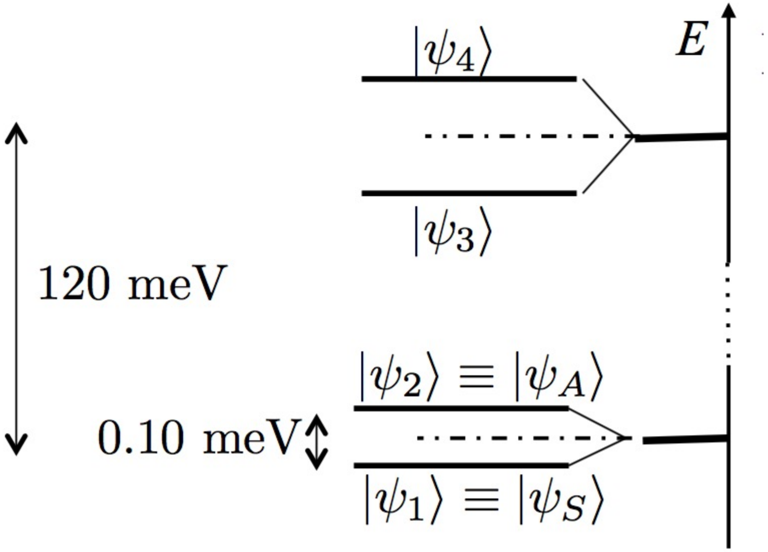


Frequency and wavelength

$$\nu_0 = \omega_0/(2\pi) = 24 \text{ GHz}$$

$$\lambda_0 = c/\nu_0 = 1.25 \text{ cm}$$

Position operator

Consider the following matrix elements

In the basis

$$(|\varphi_A\rangle\,,|\varphi_S\rangle)$$

$$\langle\psi_A|\hat{X}|\psi_A\rangle = \int x\,|\,\varphi_A\,|^2\,dx = 0$$

$$\langle\psi_S|\hat{X}|\psi_S\rangle = \int x\,|\,\varphi_S\,|^2\,dx = 0$$

$$\langle\psi_A|\hat{X}|\psi_S\rangle = \int \varphi_A^* x \varphi_S\,dx = x_0$$

$$\langle\psi_S|\hat{X}|\psi_A\rangle = \int \varphi_S^* x \varphi_A\,dx = x_0$$

Parity

+

Real functions

$$\hat{X} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} 0 & x_0 \\ x_0 & 0 \end{pmatrix}$$

It is not a position but rather a disposition with respect to the center (non-diagonal operator)

Position operator

Let us determine the eigenvalues and eigenvectors

$$\begin{pmatrix} 0 & x_0 \\ x_0 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \qquad \hat{X}\,|\varphi\rangle = \lambda\,|\varphi\rangle$$

$$\begin{vmatrix} -\lambda & x_0 \\ x_0 & -\lambda \end{vmatrix} = 0 \quad \Rightarrow \quad \lambda = \pm x_0$$

and

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

$$\frac{1}{\sqrt{2}}\left(|\varphi_A\rangle + |\varphi_S\rangle\right) = |\varphi_D\rangle$$

$$\frac{1}{\sqrt{2}}\left(|\varphi_A\rangle - |\varphi_S\rangle\right) = |\varphi_G\rangle$$

In the basis $\left(|\varphi_D\rangle, |\varphi_G\rangle\right)$ the position operator is a diagonal with eigenvectors that are linear combinations of A and S quantum states

Time evolution

We have see that if $|\psi(t=0)\rangle = |\varphi_D\rangle = \frac{1}{\sqrt{2}}(|\varphi_A\rangle + |\varphi_S\rangle)$

Then, we get $|\psi(t)\rangle = \cos\left(\frac{\omega_0 t}{2}\right)|\varphi_D\rangle + i\sin\left(\frac{\omega_0 t}{2}\right)|\varphi_G\rangle$

$$P(D) = |\langle\varphi_D|\psi(t)\rangle|^2 = \cos^2\left(\frac{\omega_0 t}{2}\right)$$

$$P(G) = |\langle\varphi_G|\psi(t)\rangle|^2 = \sin^2\left(\frac{\omega_0 t}{2}\right)$$

$$\langle\psi(t)|\hat{X}|\psi(t)\rangle = x_0 P(D) - x_0 P(G) = x_0\cos(\omega_0 t)$$

The expectation value of the position operator oscillates over time hence which proves the motion of inversion of the molecule

Quiz n°4

In "Right" (D) and "Left"(G) states, what is the dispersion ΔX of the position operator?

1. **$\Delta X = 0$**

2. **$\Delta X = x0$**

3. **$\Delta X = x0/\sqrt{2}$**

In this basis, the operator is diagonal and the eigenvectors are linear combinations of the symmetric and anti-symmetric quantum states

Quiz n°4

In “Right” (D) and “Left”(G) states, what is the dispersion ΔX of the position operator?

1. $\boxed{\Delta X = 0}$

2. $\Delta X = x0$

3. $\Delta X = x0/\sqrt{2}$

Interference & measurement

Suppose we start with an energy eigenstate $|\varphi_S\rangle$

$$|\varphi_S\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_D\rangle + |\varphi_G\rangle\right)$$

If we measure X, we can find ± x_0 with probabilities 1/2

Suppose the measurement has given the result +x_0; the state right after the measurement is then

$$|\varphi_D\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_S\rangle + |\varphi_A\rangle\right)$$

If we measure X again immediately afterwards, before the oscillation is appreciable, we find +x_0 with probability 1; the state after the measurement is $|\varphi_D\rangle$

Interference & measurement

Now, suppose that, on this new state $|\varphi_D\rangle$ we measure not X but the energy E which we are sure was E = E_S when we started. We know that that we do not always find E_S but the two possibilities E_S and E_A, each with a probability of 1/2

→ We see in this case how the measurement has perturbed the system

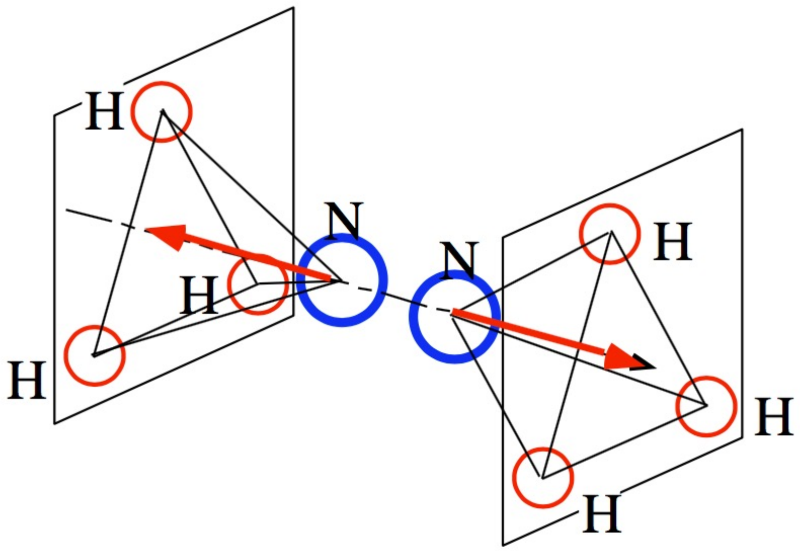
At the beginning, the state was $|\varphi_S\rangle$

At the end it is a mixture of $|\varphi_S\rangle$ and $|\varphi_A\rangle$ in interference, for which $\langle E \rangle = (E_S + E_A)/2$

All of this results from the superposition principle on one hand and the filtering of which a measurement consists

→A position measurement implies a minimum energy exchange with the system. Here, on the average, the exchange of energy is equal to A

Ammonia in an electric field



Static electric field E

Permanent electric dipole $\hat{D} = q\hat{X}$

Interaction energy with the field

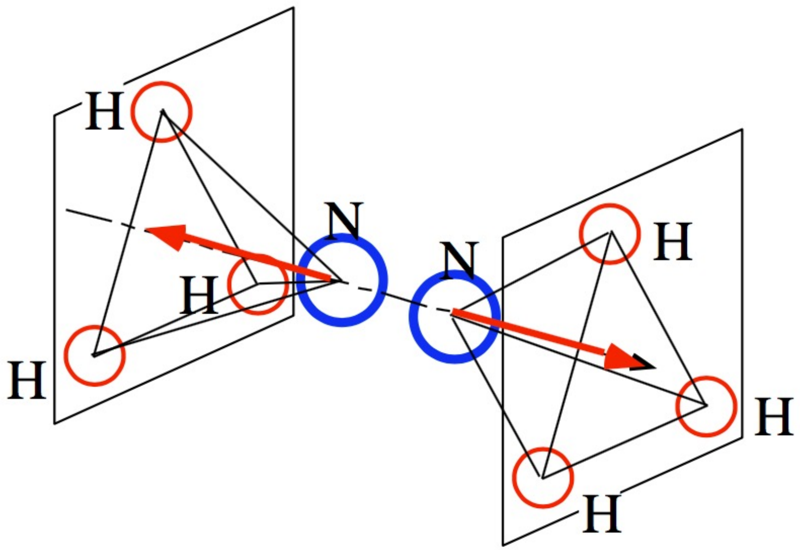
$$\hat{W} = -\hat{D}.E = \frac{\hbar}{2}\begin{pmatrix} 0 & \xi \\ \xi & 0 \end{pmatrix}$$

$$\frac{\hbar}{2}\xi = -qx_0E = -d_0E$$

In other words, if we measure X and we find $\pm x_0$ with some probabilities, a measurement of D will give $\pm d_0$ with the same probabilities
The only difficulty, here, is to accept that a good model for the observable D, is to be proportional to X

The potential energy observable W is simply the product of the observable D by the numerical value of the applied electric field. The only real justification for this choice is that it works very well

Ammonia in an electric field



Static electric field E

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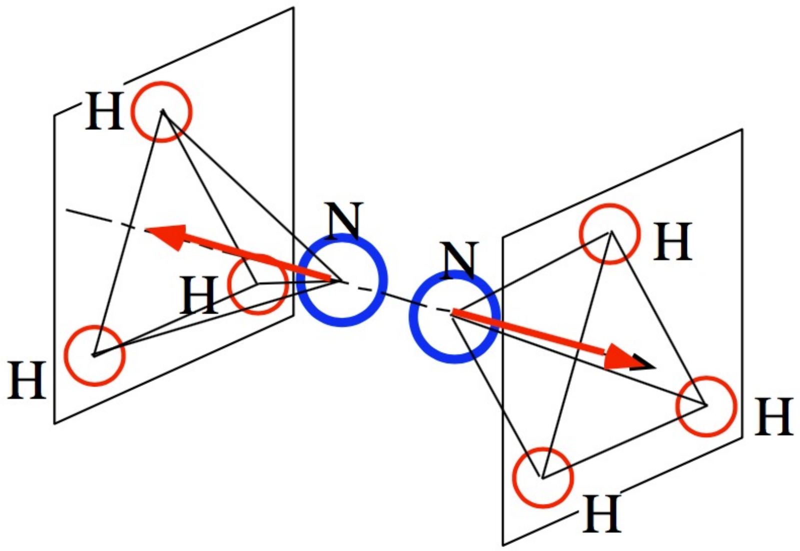
$$\frac{\hbar}{2}\xi = -qx_0E = -d_0E$$

When the nitrogen flips from one side to the other, the center of mass will not move, but the electric dipole moment will flip over

$$\hat{H}_{NH_3} = \begin{pmatrix} E_A & 0 \\ 0 & E_S \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

$$\hat{H} = H_{NH_3} + \hat{W} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \xi \\ \xi & -\omega_0 \end{pmatrix}$$

Ammonia in an electric field



Static electric field E

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$$\hat{H}_{NH_3} = \begin{pmatrix} E_A & 0 \\ 0 & E_S \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}$$

$$\hat{H} = H_{NH_3} + \hat{W} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \xi \\ \xi & -\omega_0 \end{pmatrix}$$

Ammonia in an electric field

Eigenvalues

$$\begin{vmatrix} \omega_0 - \lambda & \xi \\ \xi & -\omega_0 - \lambda \end{vmatrix} = 0$$

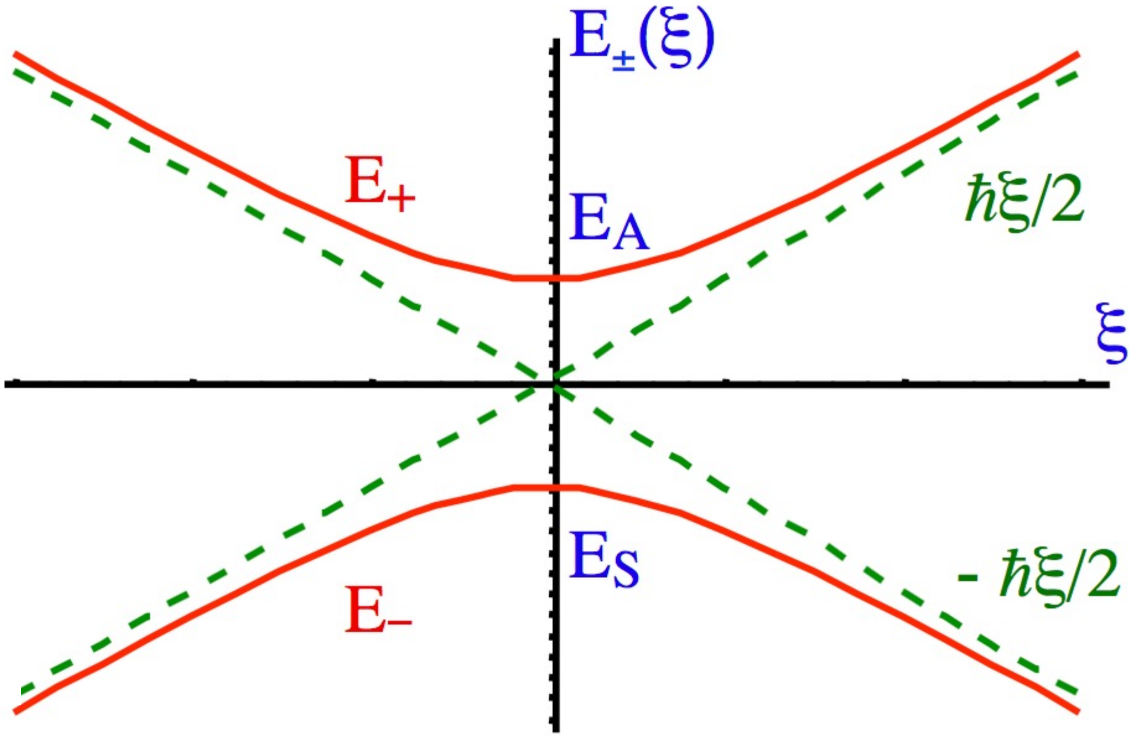
$$\lambda^2 - \omega_0^2 - \xi^2 = 0$$

$$\lambda_\pm = \pm\sqrt{\omega_0^2 + \xi^2}$$

$$E_\pm = \pm\frac{\hbar}{2}\sqrt{\omega_0^2 + \xi^2}$$

$$\hbar\omega_0 = E_A - E_S$$

$$\hbar\xi = -2d_0E$$



Ammonia in an electric field

Eigenvectors

$$\cos(\theta) = \frac{\omega_0}{\sqrt{{\omega_0}^2 + \xi^2}} \qquad \sin(\theta) = \frac{\xi}{\sqrt{{\omega_0}^2 + \xi^2}}$$

$$\boxed{|\varphi_+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \qquad |\varphi_-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}}$$

which can be expressed as

$$|\varphi_+\rangle = \cos(\theta/2)\,|\varphi_A\rangle + \sin(\theta/2)\,|\varphi_S\rangle$$

$$|\varphi_-\rangle = -\sin(\theta/2)\,|\varphi_A\rangle + \cos(\theta/2)\,|\varphi_S\rangle$$

$$|\varphi_S\rangle = \sin(\theta/2)\,|\varphi_+\rangle + \cos(\theta/2)\,|\varphi_-\rangle$$

$$|\varphi_A\rangle = \cos(\theta/2)\,|\varphi_+\rangle - \sin(\theta/2)\,|\varphi_-\rangle$$

Ammonia in an electric field

Eigenvectors

$$\cos(\theta) = \frac{\omega_0}{\sqrt{\omega_0^{\,2} + \xi^2}} \qquad \sin(\theta) = \frac{\xi}{\sqrt{\omega_0^{\,2} + \xi^2}}$$

$$\boxed{|\varphi_+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \qquad |\varphi_-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}}$$

Time evolution

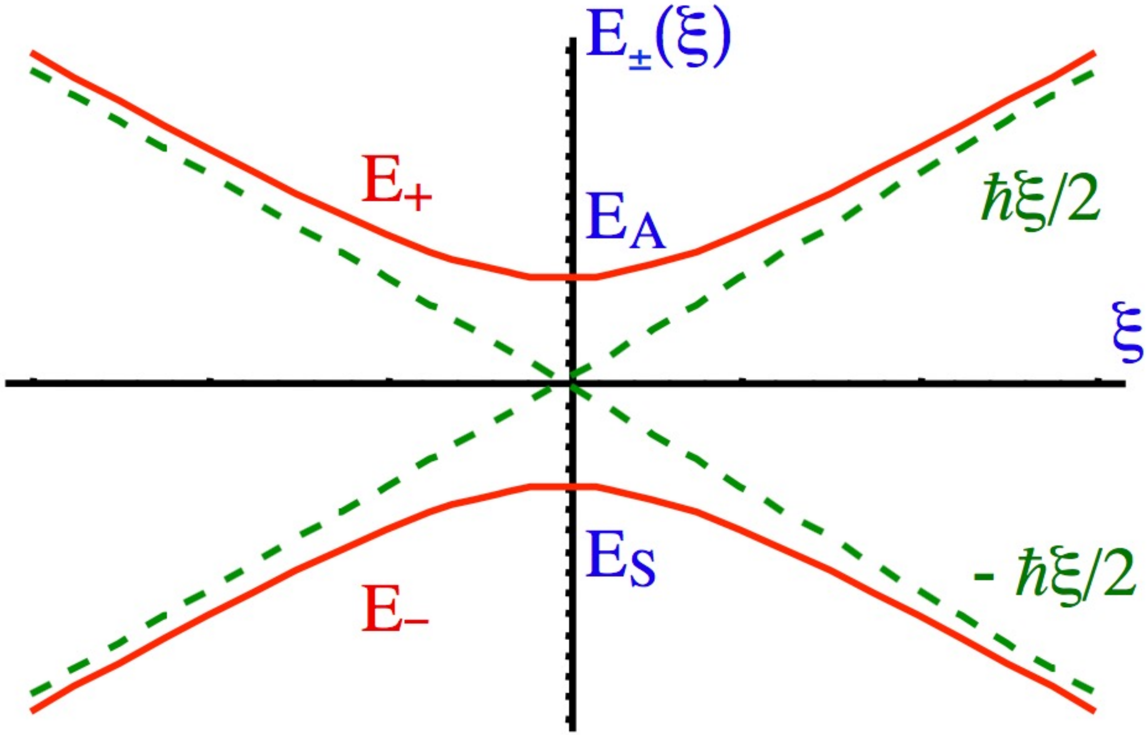
$$|\varphi(t=0)\rangle = |\varphi A\rangle = \cos(\theta/2)|\varphi_+\rangle - \sin(\theta/2)|\varphi_-\rangle$$

$$|\varphi(t)\rangle = \cos(\theta/2)\, e^{-iE_+t/\hbar}|\varphi_+\rangle - \sin(\theta/2)\, e^{-iE_-t/\hbar}|\varphi_-\rangle$$

Probability $|\langle\varphi_S|\varphi(t)\rangle|^2$ of switching from A to S

$$\boxed{P(A \to S) = \sin^2(\theta)\sin^2\frac{(E_+ - E_-)t}{2\hbar} = \frac{\xi^2}{\omega_0^{\,2} + \xi^2}\sin^2\frac{\sqrt{\omega_0^{\,2} + \xi^2}\; t}{2}}$$

Ammonia in an electric field



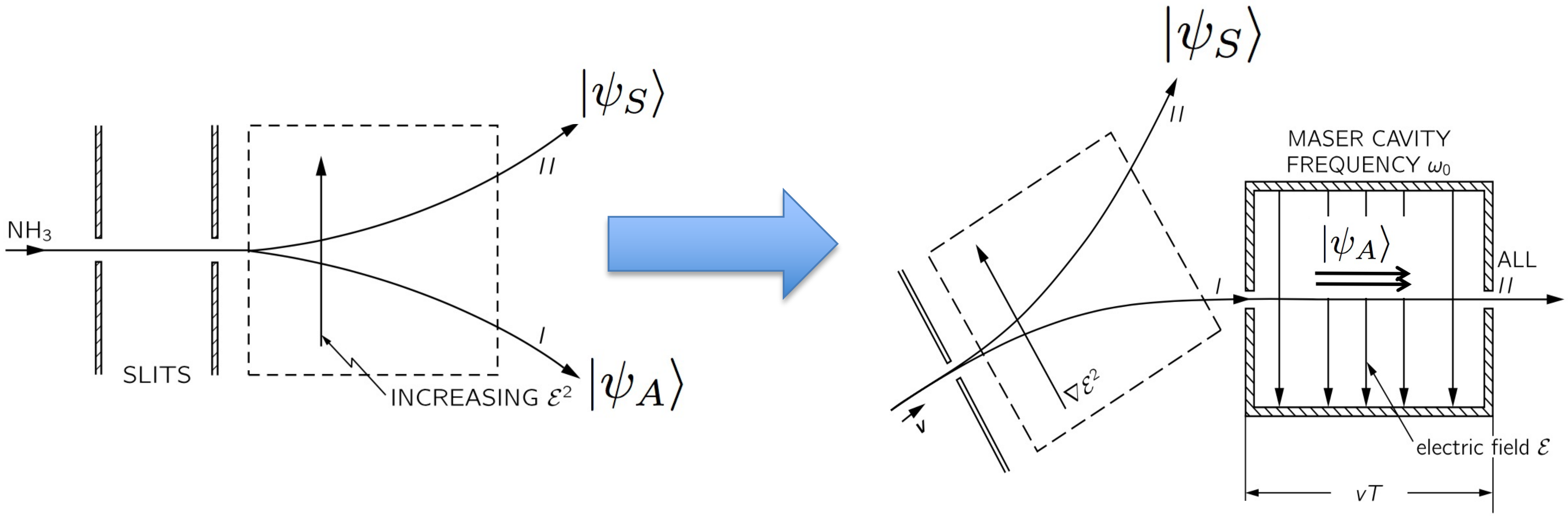
Consider the two limiting cases:

→ **Weak field effect ($\vartheta << 1$), the tunneling effect tends to symmetrize the molecule, which results in a vanishing dipole moment <D> = 0**

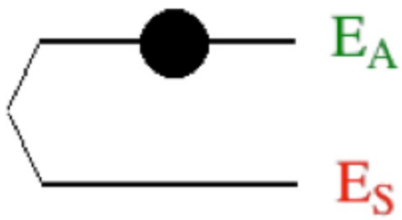
→ **Strong field effect ($\vartheta = \pi/2$) pulls the molecule toward the classical configurations D and G ("Right" and "Left") where it has a dipole moment <D> = ± d_0**

Ammonia in an inhomogeneous electric field

The ammonia gas is simply let out of a little jet and passed through a pair of slits to give a narrow beam. The beam is then sent through a region in which there is a large transverse electric field

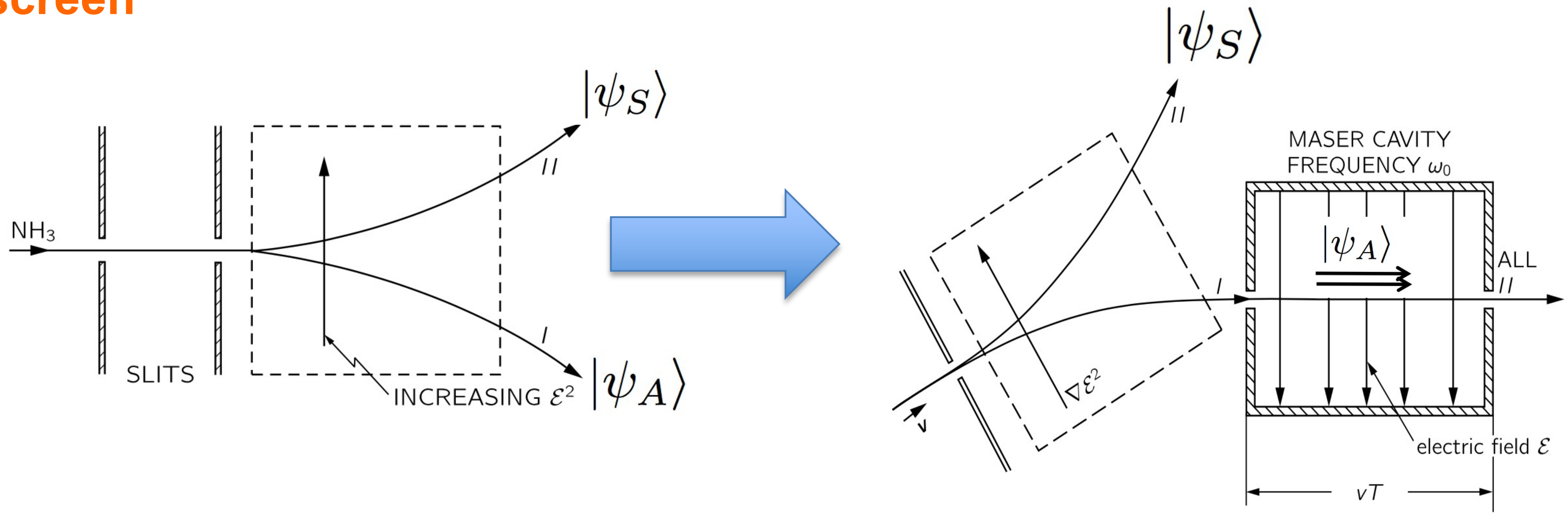


We have reached population inversion
At the output, the system is out of the equilibrium



Ammonia in an inhomogeneous electric field

Here we face an incredible phenomenon. There are only two quantum trajectories whereas classically, if the electric dipole moments were oriented at random there should be a continuous set of impacts on a screen



This apparatus is a concrete example of a quantum mechanical measuring apparatus. It transfers internal quantum degrees of freedom into classical space properties. It is also a device to prepare the molecules in the states S or A , or in linear superpositions of them

Reaction to an oscillating electric field

Interaction energy between the dipole and the field

$$\hat{W} = -\hat{D}E_0\cos(\omega t) = \hbar\begin{pmatrix} 0 & \xi_0\cos(\omega t) \\ \xi_0\cos(\omega t) & 0 \end{pmatrix}$$

leading to

$$\hat{H} = \hbar\begin{pmatrix} \omega_0/2 & \xi_0\cos(\omega t) \\ \xi_0\cos(\omega t) & -\omega_0/2 \end{pmatrix}$$

Here we have time dependent Schrödinger equation hence the standard method does not apply anymore!!

Rotating wave approximation: Terms in a Hamiltonian which oscillate rapidly can be neglected. This is a valid approximation as long as the applied electromagnetic radiation takes place near the resonance with an atomic transition, as well as the intensity is low

Reaction to an oscillating electric field

Time dependent Shrödinger's equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \quad \Rightarrow \quad i\hbar \frac{d}{dt}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} = \hat{H}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix}$$

leading to

$$i\frac{d\alpha}{dt} = \frac{\omega_0}{2}\alpha(t) + \xi_0\cos(\omega t)\beta(t)$$

$$i\frac{d\beta}{dt} = \frac{-\omega_0}{2}\beta(t) + \xi_0\cos(\omega t)\alpha(t)$$

Consider the substitution

$$\alpha(t) = \tilde{\alpha}(t)e^{-i\omega t/2}$$

$$\beta(t) = \tilde{\beta}(t)e^{i\omega t/2}$$

Reaction to an oscillating electric field

Time dependent Shrödinger's equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \quad \Rightarrow \quad i\hbar \frac{d}{dt} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix} = \hat{H} \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix}$$

The substitution leads to

$$i\frac{d\tilde{\alpha}}{dt} = (-\omega + \omega_0)\tilde{\alpha}(t)/2 + \xi_0(1 + e^{2i\omega t})\tilde{\beta}(t)/2$$

$$i\frac{d\tilde{\beta}}{dt} = (\omega - \omega_0)\tilde{\beta}(t)/2 + \xi_0(1 + e^{-2i\omega t})\tilde{\alpha}(t)/2$$

with $\delta = \omega - \omega_0$

Using the rotating wave approximation, fast oscillations terms are neglected in the above equations → solutions are analytically extracted

Reaction to an oscillating electric field

Time dependent Shrödinger's equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \quad \Rightarrow \quad i\hbar \frac{d}{dt}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} = \hat{H}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix}$$

The substitution leads to

$$i\frac{d\tilde{\alpha}}{dt} = (-\omega + \omega_0)\tilde{\alpha}(t)/2 + \xi_0(1 + \cancel{e^{2i\omega t}})\tilde{\beta}(t)/2$$

$$i\frac{d\tilde{\beta}}{dt} = (\omega - \omega_0)\tilde{\beta}(t)/2 + \xi_0(1 + \cancel{e^{-2i\omega t}})\tilde{\alpha}(t)/2$$

with $\delta = \omega - \omega_0$

Using the rotating wave approximation, fast oscillations terms are neglected in the above equations → solutions are analytically extracted

Reaction to an oscillating electric field

Time dependent Shrödinger's equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \quad \Rightarrow \quad i\hbar \frac{d}{dt}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix} = \hat{H}\begin{pmatrix}\alpha(t)\\ \beta(t)\end{pmatrix}$$

Then we get

$$\frac{d^2\tilde{\alpha}}{dt^2} + \Omega_0^2\tilde{\alpha} = 0$$

$$\frac{d^2\tilde{\beta}}{dt^2} + \Omega_0^2\tilde{\beta} = 0$$

with

$$\Omega_0 = \frac{1}{2}\sqrt{\delta^2 + \xi_0^2}$$

Consider the initial conditions

$$\beta(t=0) = 0$$

Then we get

$$\tilde{\beta}(t) = -i\frac{\xi_0}{2\Omega_0}\sin(\Omega t)$$

$$\tilde{\alpha}(t) = \cos(\Omega_0 t) + i\frac{\delta}{2\Omega_0}\sin(\Omega_0 t)$$

$$|\psi(t)\rangle = \tilde{\alpha}(t)|\alpha\rangle + \tilde{\beta}(t)|\beta\rangle$$

Reaction to an oscillating electric field

Probability of switching from A to S

$$P(A \to S) = |\langle \tilde{\beta} | \psi \rangle|^2 = |\tilde{\beta}(t)|^2 = |\beta(t)|^2$$

$$\mathrm{P}(\mathrm{A} \to \mathrm{S}) = \frac{\xi_0^2}{(\omega - \omega_0)^2 + \xi_0^2} \sin^2 \frac{\sqrt{(\omega - \omega_0)^2 + \xi_0^2}\, t}{2}$$

with an oscillating electric field with frequency ω applied from 0 to t

And with a static electric field applied from 0 to time t, we retrieve as in pp. 198

$$\mathrm{P}(\mathrm{A} \to \mathrm{S}) = \frac{\xi^2}{\omega_0^2 + \xi^2} \sin^2 \frac{\sqrt{\omega_0^2 + \xi^2}\, t}{2}$$

Rabi's formula (resonant excitation obtained for $\delta = \omega - \omega_0 = 0$)

Reaction to an oscillating electric field

Probability of switching from A to S

Rabi's formula

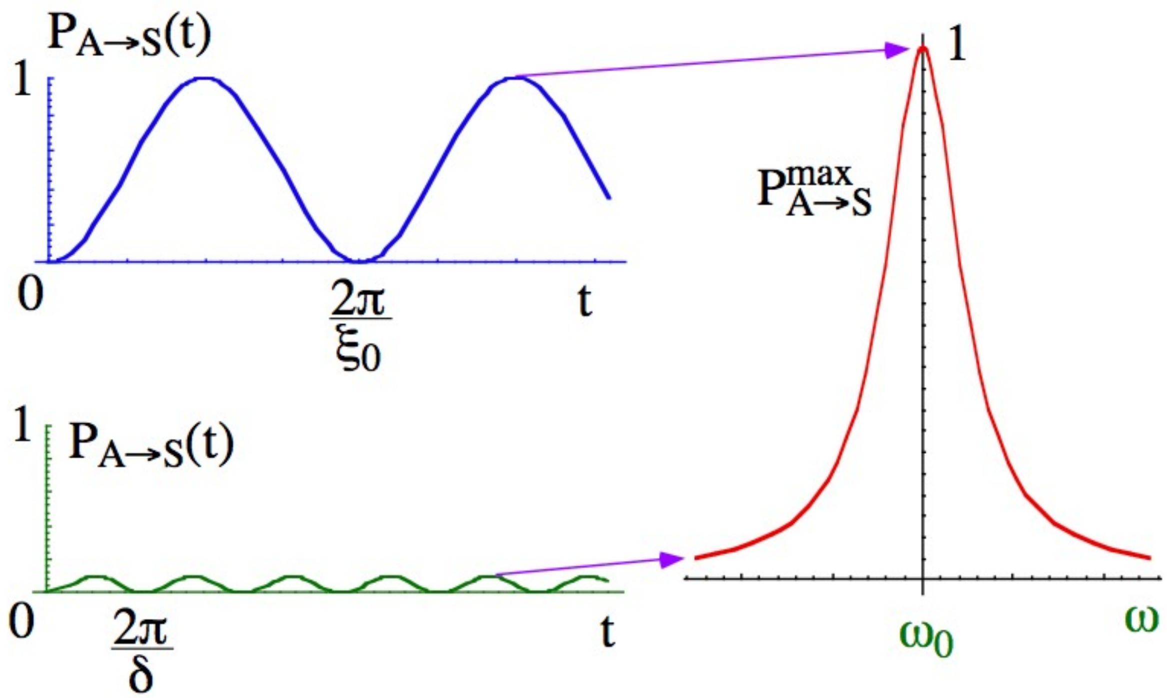
$$P(A \to S) = \frac{\xi_0^2}{(\omega-\omega_0)^2+\xi_0^2}\sin^2\frac{\sqrt{(\omega-\omega_0)^2+\xi_0^2}\;t}{2}$$

$\omega = \omega_0$

$$P_{A\to S}(t) = \sin^2\left(\xi_0 \frac{t}{2}\right)$$

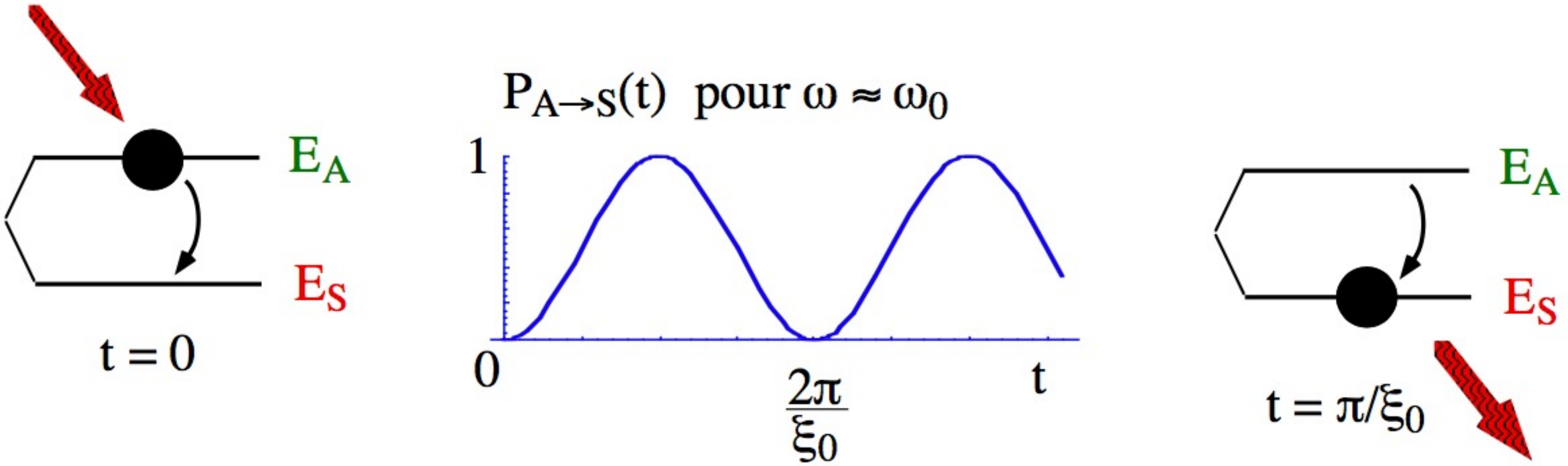
$\delta = \omega - \omega_0$, $|\delta| >> \xi_0$

$$P_{A\to S}(t) = \frac{\xi_0^2}{\delta^2}\sin^2\left(\delta \frac{t}{2}\right)$$



Stimulated emission

Molecule in a state A with energy E_A in interaction with an electric field oscillating at ω_0

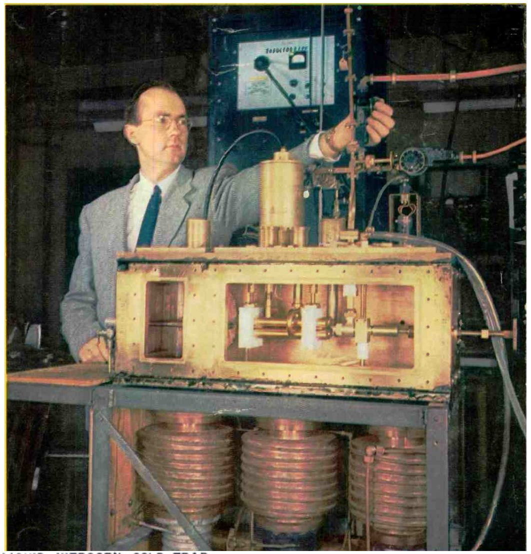


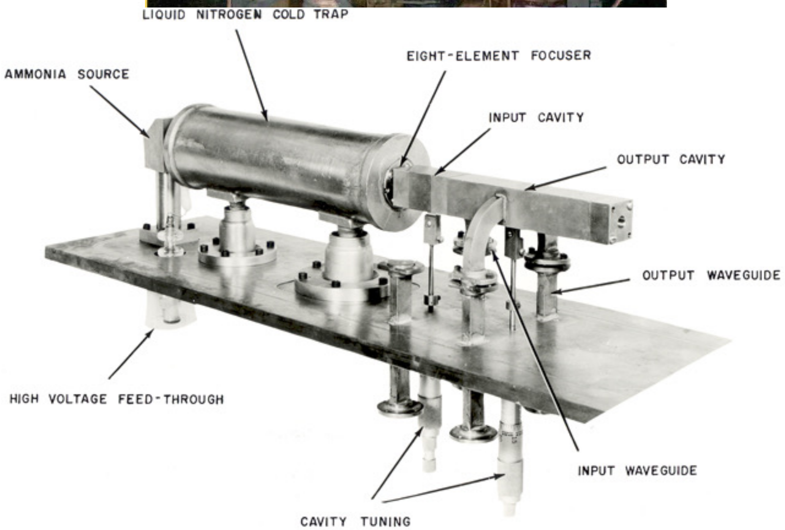
- → **The field induces the stimulated emission of the molecule**
- → **Then, the molecule yields its energy to the field. If the field is confined in a cavity, the process is reversible**
- → **The field at the outside the cavity is greatly amplified**

Amplification by stimulated emission of radiation
MASER & LASER

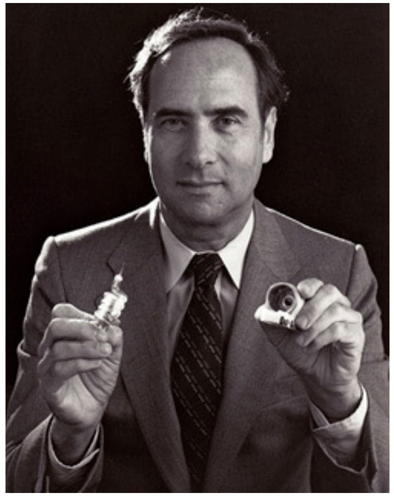
Maser & Laser

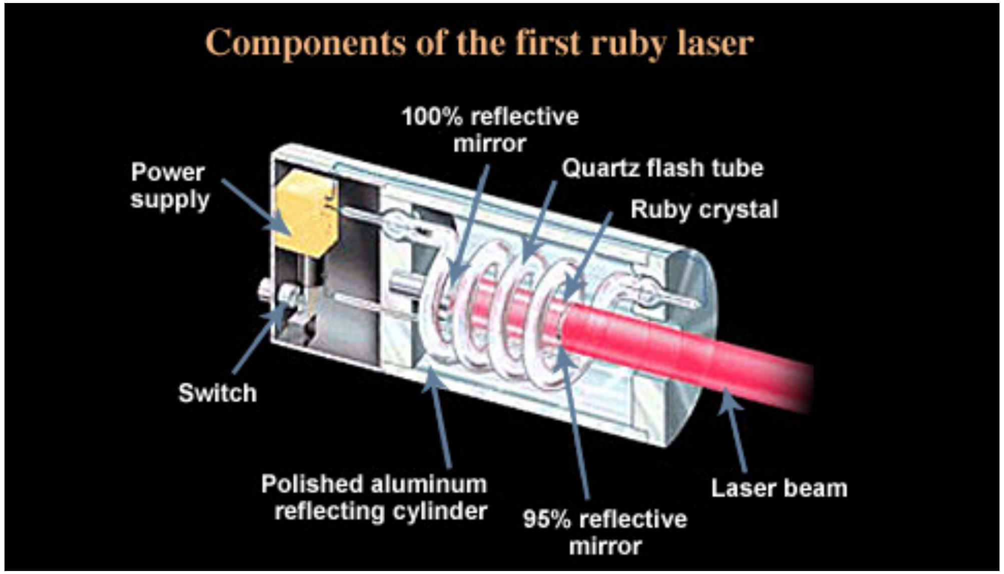
First Maser (C. Townes, 1954)
P=10^{-9} W, f=24 GHz (microwave)



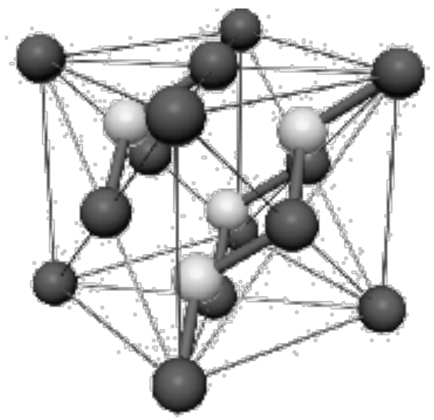


First Laser (T. Maiman, 1960)



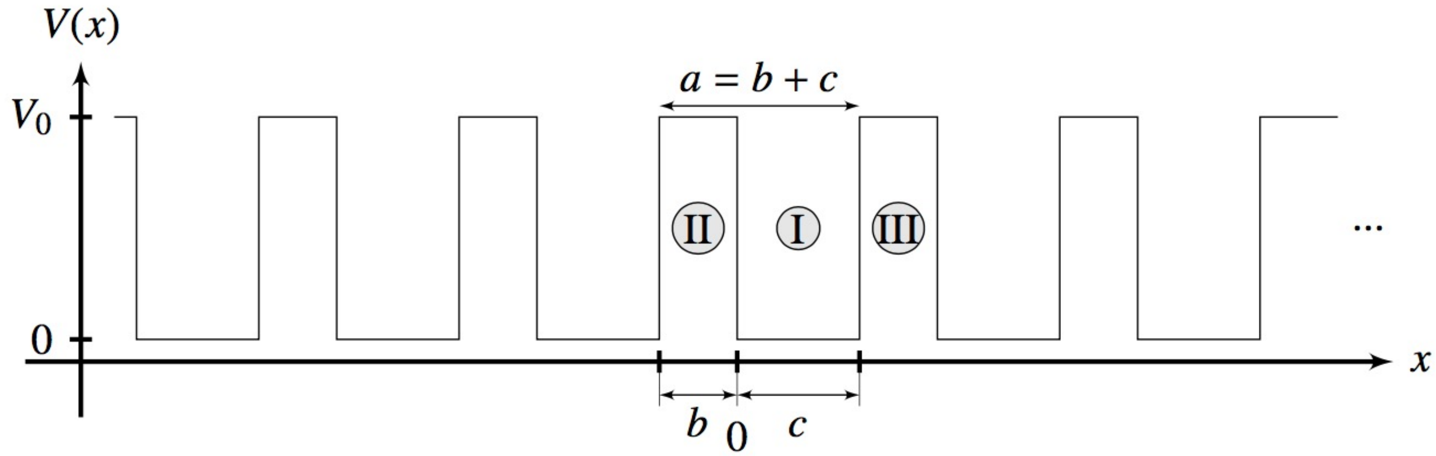


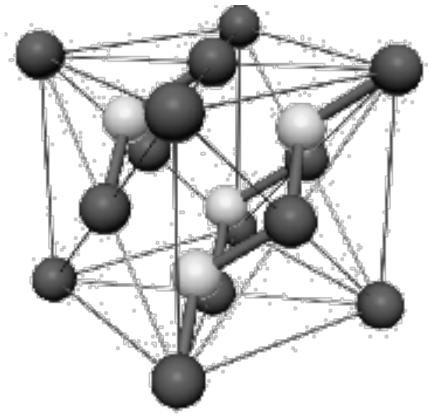
4.
Electrons in solids



Electrons in solids

The Kronig-Penney model demonstrates that a simple one-dimensional periodic potential yields energy bands as well as energy band gaps





Bloch wave

$$\psi(x) = u_k(x)\, e^{ikx}$$

$$k \in \left[-\frac{\pi}{a}; -\frac{\pi}{a}\right]$$

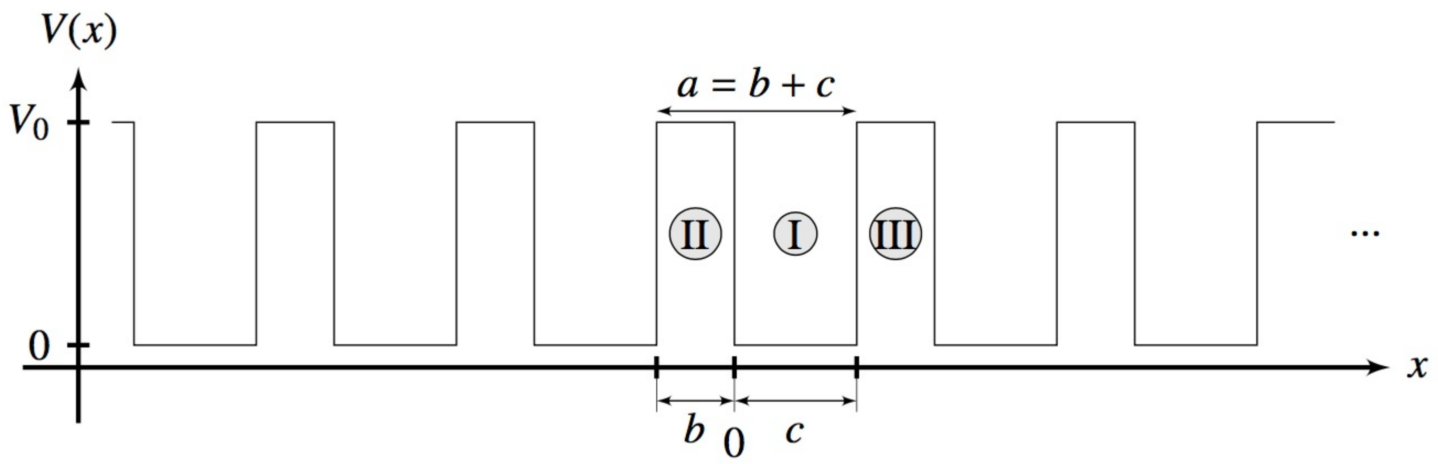
Double periodicity

$$u_k(x+a) = u_k(x)$$

$$u_{k+\frac{2\pi}{a}} = u_k$$

Bloch's theorem: The energy eigenstates for an electron in a crystal can be written as Bloch waves i.e. the electron wave functions in a crystal have a basis consisting entirely of Bloch wave energy eigenstates

Electrons in solids



Consider the solutions of the Schrödinger's equation in regions I, II and III

$$0 \leqslant x < c \qquad \psi(x) = \psi_I(x) = Ae^{i\alpha x} + Be^{-i\alpha x} \qquad \alpha^2 = \frac{2m}{\hbar^2}E \qquad (1a)$$

$$-b \leqslant x < 0 \qquad \psi(x) = \psi_{II}(x) = Ce^{i\beta x} + De^{-i\beta x} \qquad \beta^2 = \frac{2m}{\hbar^2}(E - V_0) \qquad (1b)$$

$$c \leqslant x < a \qquad \psi(x) = \psi_{III}(x) = C'e^{i\beta x} + D'e^{-i\beta x} \quad C' = Ce^{i(k-\beta)a}, D' = De^{i(k+\beta)a} \qquad (1c)$$

Electrons in solids

Boundary conditions (continuity and derivatives x=0 and x=c)

$$A + B = C + D$$
$$\alpha A - \alpha B = \beta C - \beta D$$
$$A e^{i\alpha c} + B e^{-i\alpha c} = C e^{ika} e^{-i\beta b} + D e^{ika} e^{i\beta b}$$
$$\alpha A e^{i\alpha c} - \alpha B e^{-i\alpha c} = \beta C e^{ika} e^{-i\beta b} - \beta D e^{ika} e^{i\beta b}$$

We can express the general solution as follows

$$\cos(ka) = \cos(\alpha c) \cdot \cos(\beta b) - \frac{\alpha^2 + \beta^2}{2\alpha\beta} \cdot \sin(\alpha c) \cdot \sin(\beta b)$$

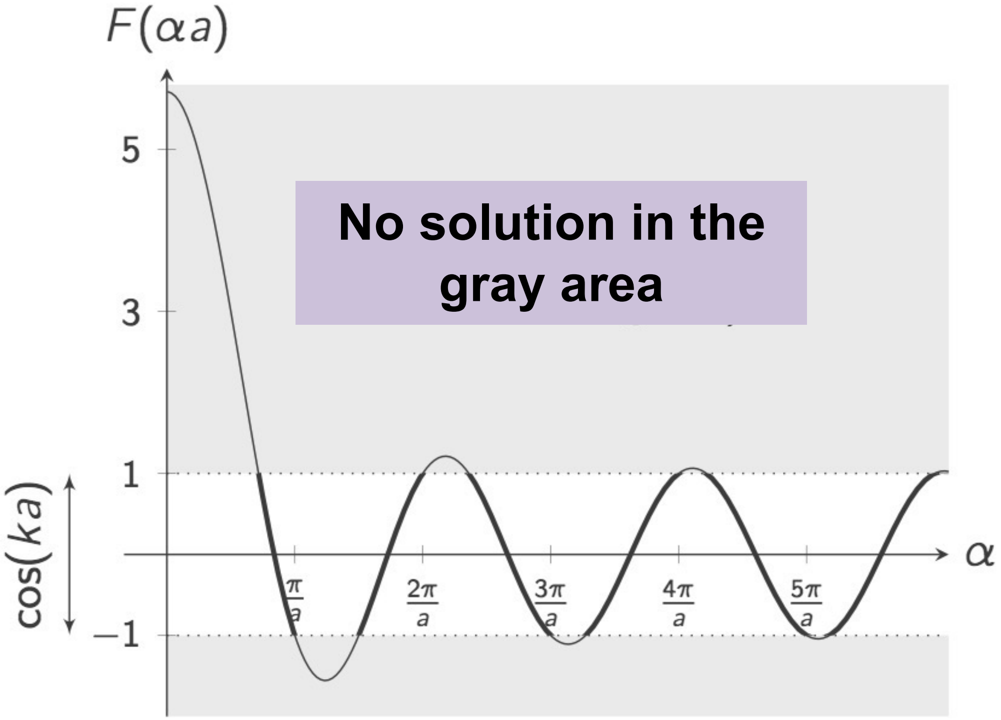
Consider the following conditions: We search bound states and assume narrow barrier, and strong tunneling

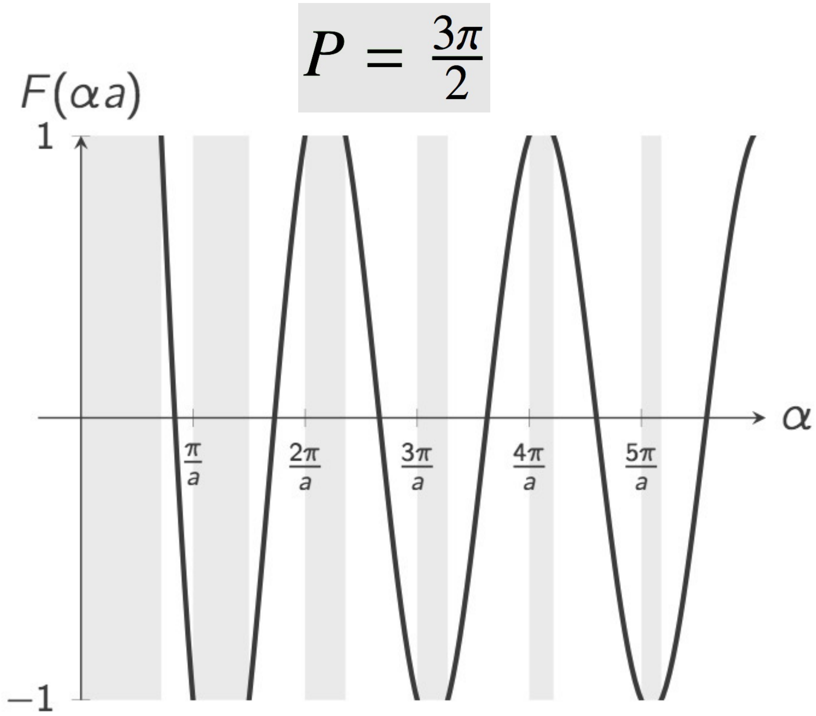
$$V_0 \gg E \qquad b \ll a, c \simeq a \qquad |\beta b| \ll 1$$

$$\Rightarrow \quad \cos(ka) = \cos(\alpha a) + P\frac{\sin(\alpha a)}{\alpha a} \quad \text{with} \quad P = \frac{mV_0 ab}{\hbar^2}$$

Electrons in solids

$$\cos(ka) = F(\alpha a) \quad \textbf{with} \quad F(\alpha a) = \cos(\alpha a) + P\frac{\sin(\alpha a)}{\alpha a}$$

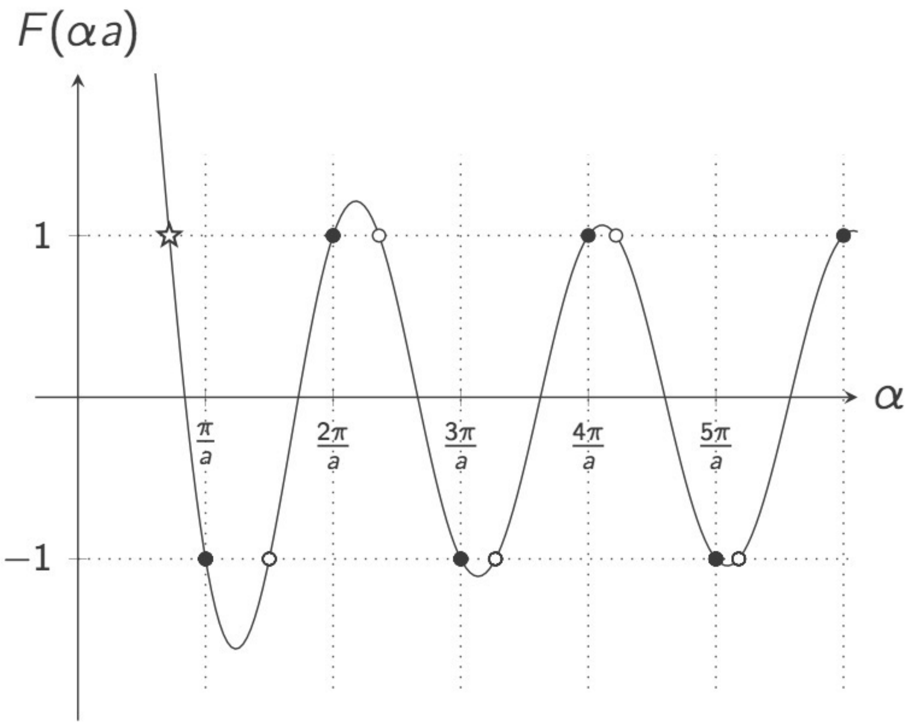


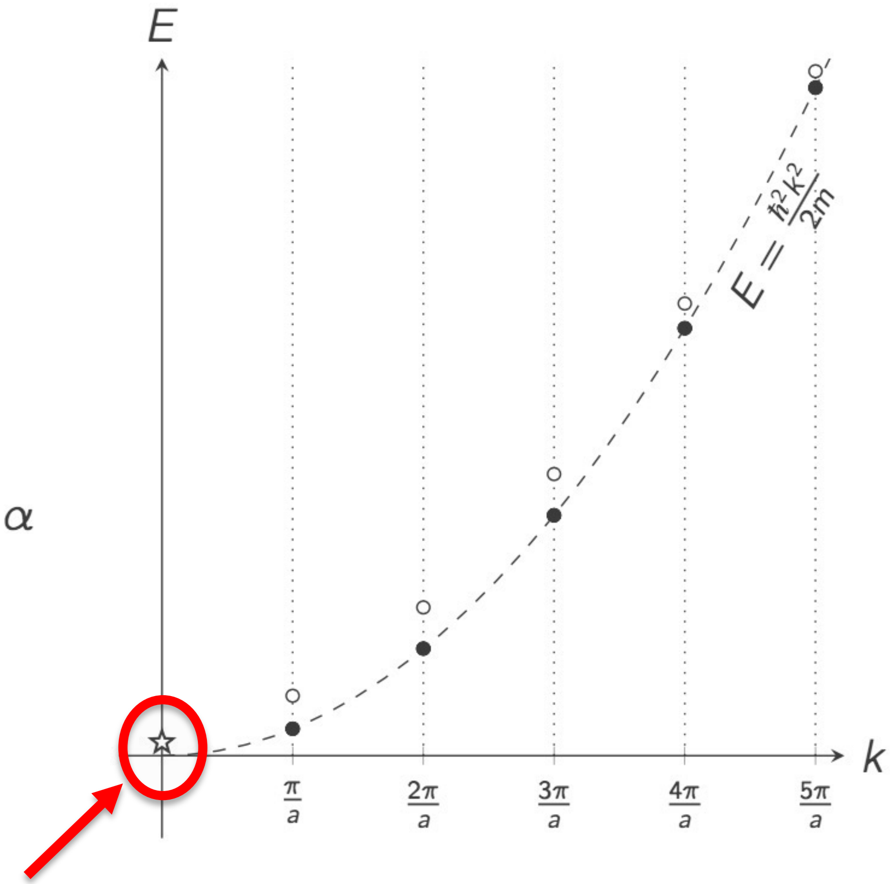


Only allowed energies are those for which −1 ≤ F(αa) ≤ 1
Whenever F(αa) is outside the domain [−1, 1], there are no solutions

Electrons in solids

Solving equation for k, we see the dependence of the energy and the formation of allowed and forbidden energy bands

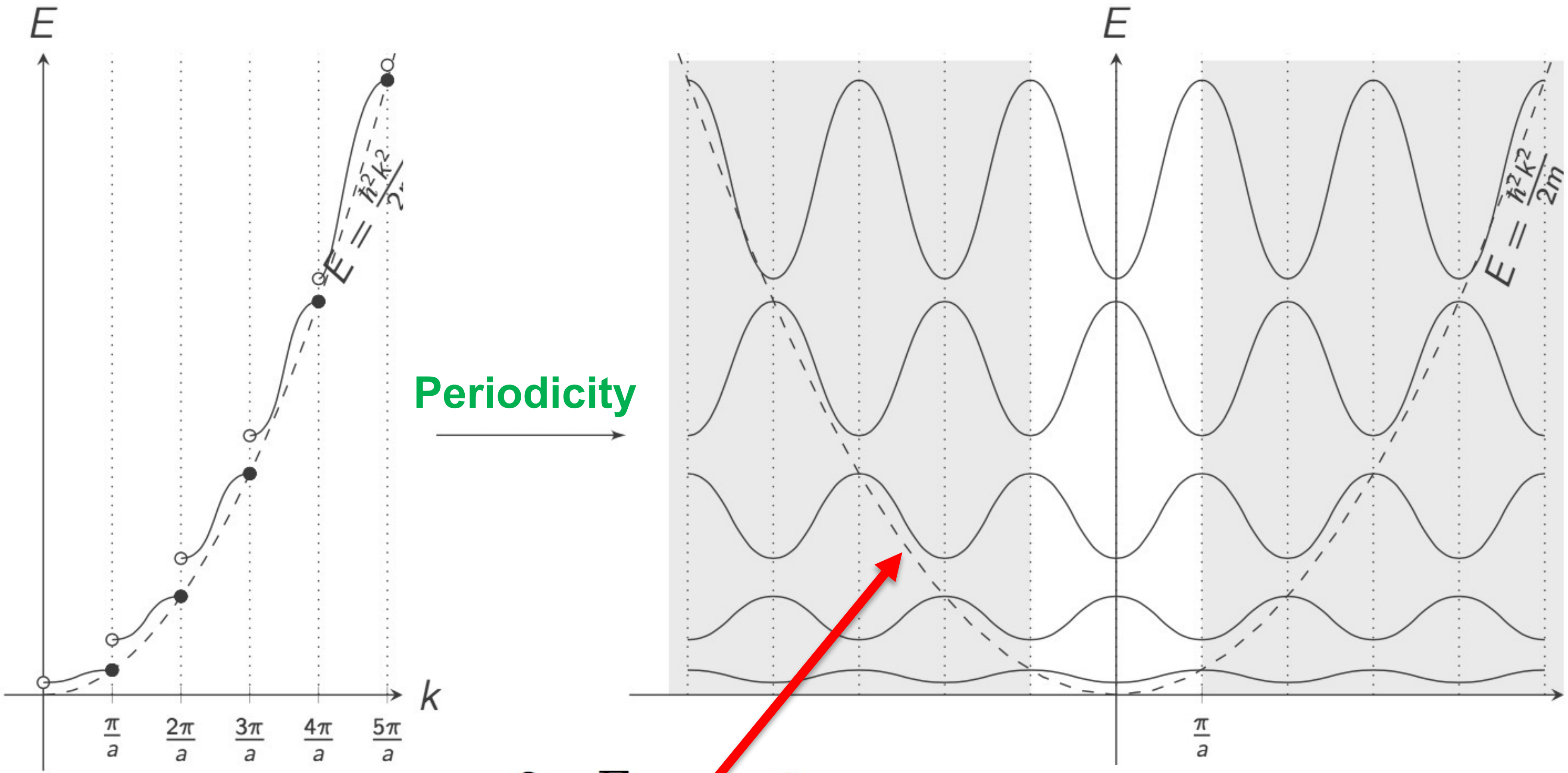




For k=0, we can find a non-zero energy as for a particle confined in a box

Electrons in solids

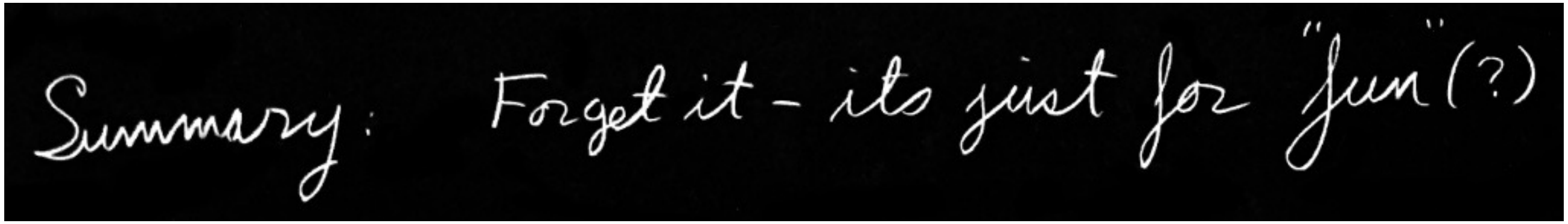
Solving for k we see the dependence of the energy and the formation of bands. Notice that a gap opens in the energy spectrum at $k = \frac{\pi}{a} n$



$$\frac{2mE}{\hbar^2} = k^2$$ **Free electron**

Section 6

Hilbert space, Dirac’s notations and matrix mechanics



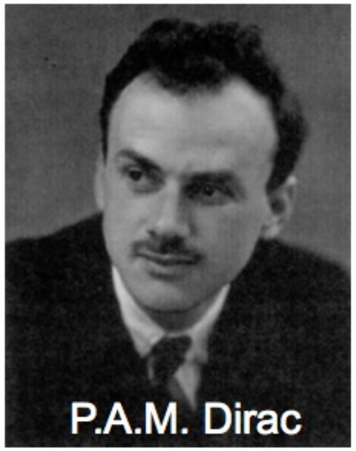
After Richard Feynman

For further information, read the supplementary material

Ket vector

Introduced by . P. A. MDirac in 1926

$$\begin{pmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \end{pmatrix} \longleftrightarrow |\psi\rangle \begin{array}{l} \nearrow\!\!\!\swarrow \ \psi(x) \\ \searrow\!\!\!\nwarrow \ \varphi(p) \end{array}$$



1933

The ket is a normed vector that is an element of an abstract complex vector space e.g. the infinite-dimensional vector space of square integrable wavefunctions

Hilbert space

A Hilbert space $\mathcal{E}_H$ is a linear vector space whose elements are functions or vectors $|\psi\rangle$ with a positive-definite scalar product

The dimensionality of the Hilbert space is the number of linearly independent vectors/states needed to span it (may be finite or infinite)

Properties

1. Linearity: if $|\psi\rangle$ and $|\phi\rangle$ are elements of $\mathcal{E}_H$ so is $a\psi + b\phi$.
2. Inner product: $\langle\psi|\phi\rangle$ exists and $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$.
3. Every element $|\psi\rangle$ has a norm/length $\|\psi\|$ such that $\langle\psi|\psi\rangle = \|\psi\|^2$.
4. Completeness: every Cauchy series of functions in $\mathcal{E}_H$ converges to an element in $\mathcal{E}_H$

Hilbert space

The Hilbert space $\mathcal{L}_2(a,b)$ is the set of all square-integrable functions f(x) on the interval [a,b], i.e., f(x) such that

$$\int_a^b f^*(x)f(x)dx < \infty$$

Inner product in

$$\langle\psi|\phi\rangle = \int_a^b \psi^*(x)\phi(x)dx$$

Note the infinite dimensionality of the Hilbert spaces (evidenced by the infinite number of energy eigenfunctions, which comprise possible bases for these spaces)

$$\mathcal{L}_2(-\infty,\infty)$$

Free particle

$$\mathcal{L}_2(0,a)$$

Infinite square well

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Generalization of the 1st postulate

Every physical system can be represented by a unique Hilbert's space $\mathcal{E}_H$

The state of a given physical system is described by a single vector state (normed vector) of unit length in the system's Hilbert space

$$|\psi(t)\rangle$$

The Hilbert's space satisfies the principle of superposition

Existence of Hilbert's basis composed of eigenstates

$$|\psi(t)\rangle \longleftrightarrow \begin{pmatrix} C_0(t) \\ C_1(t) \\ \vdots \end{pmatrix}$$

Inner product

The inner product is defined using the braket notation

$$\langle \psi_b | \psi_a \rangle$$

→ linear with the second argument, anti-linear with the first argument

$$|\psi_a\rangle = \begin{pmatrix} C_0 \\ C_1 \\ \vdots \end{pmatrix} \qquad |\psi_b\rangle = \begin{pmatrix} D_0 \\ D_1 \\ \vdots \end{pmatrix}$$ then $$\langle \psi_b | \psi_a \rangle = \sum_n D_n^* C_n$$

All acceptable vectors for a complete description of the quantum system must be normalized

$$\sum_n |C_n|^2 = 1$$

Bra vector

The bra labeled vector is obtained by forming the row vector and complex conjugating the entries

$$|\psi_b\rangle = \begin{pmatrix} D_0 \\ D_1 \\ \vdots \end{pmatrix} \Rightarrow \langle\psi_b| = (D_0^* \ , \ D_1^* \ , \ \ldots)$$

Inner product

$$\langle\psi_b|\psi_a\rangle = \sum_n D_n^* C_n$$

$$\langle\psi_b|\psi_a\rangle = (D_0^* \ , \ D_1^* \ , \ \ldots) \begin{pmatrix} C_0 \\ C_1 \\ \vdots \end{pmatrix}$$

Braket = complex number

Matrix mechanics

An operator $\hat{A}$ is described by a matrix $[A_{p,n}]$ acting in the Hilbert's space basis $|\phi_n\rangle$

$$A_{p,n} = \underbrace{\langle\phi_p|}_{\text{Row vector}} \; \big(\underbrace{\hat{A}}_{\text{Square matrix}}\underbrace{|\phi_n\rangle}_{\text{Column vector}}\big) \qquad = \langle\phi_p|\hat{A}|\phi_n\rangle$$

Operators are Hermitian (or self-adjoints) if and only if

$$[\hat{A}^\dagger]_{p,n} = \left([\hat{A}]_{n,p}\right)^* \Rightarrow \hat{A} = \hat{A}^\dagger$$

Matrix mechanics

Examples of Hermitian operators

$$\widehat{x},\ \widehat{p}_x, \qquad \hat{A} = \begin{pmatrix} 5 & 2+3i \\ 2-3i & -1 \end{pmatrix}$$

Spectral theorem: a Hermitian matrix is diagonalizable and as a consequence it is possible to find a Hilbert's basis composed of eigenvectors

$$\hat{A}|\psi_n\rangle = a_n|\psi_n\rangle \qquad \text{such as} \qquad \langle\psi_p|\psi_n\rangle = \delta_{p,n}$$

All eigenvalues of Hermitian operators are real. Therefore, (by postulate), all operators for physical observables are Hermitian (because measured quantities are real numbers). Some subtleties persist with Hilbert's space with infinite dimensional case

The Hamiltonian

Physical quantity: energy E $\longrightarrow$ Energy operator: Hamiltonian $\widehat{H}$

hermitien

As in classical physics, possible values for the energy will depend on the physical configuration of the problem

➡ Particle of mass m in a potential

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

➡ Dipole in an external electric field (E)

$$\widehat{H} = -\widehat{\vec{D}} \cdot \vec{E}$$

➡ Dipole in an external magnetic field (B)

$$\widehat{H} = -\widehat{\vec{\mu}} \cdot \vec{B}$$

Potential energy of Interaction

Projection operator

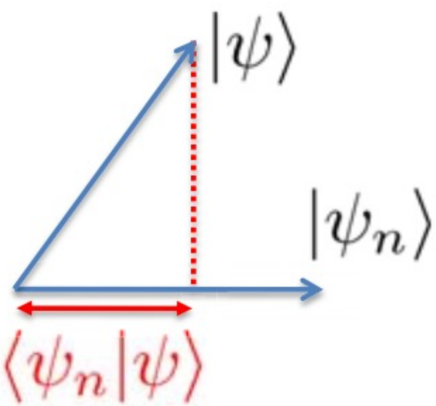
- $P_n = |\psi_n\rangle\langle\psi_n|$ **is an operator (not closed braket)**

- $P_n = |\psi_n\rangle\langle\psi_n|$ **is a projector**

$$P_n^2 = (|\psi_n\rangle\langle\psi_n|)^2 = |\psi_n\rangle\langle\psi_n|\psi_n\rangle\langle\psi_n| = |\psi_n\rangle\langle\psi_n| = P_n$$

- $P_n = |\psi_n\rangle\langle\psi_n|$ **is a projector on state** $|\psi\rangle$

$$P_n|\psi\rangle = (|\psi_n\rangle\langle\psi_n|)|\psi\rangle$$
$$= (\langle\psi_n|\psi\rangle)|\psi_n\rangle$$



Here the operator projects a vector onto the n^th eigenstate

Projection operator

$$\langle\psi_n| = \begin{pmatrix} 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{pmatrix}$$

$$|\psi_n\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \qquad |\psi_n\rangle\langle\psi_n| = \begin{pmatrix} 0 & & & & & \\ & \ddots & & & \mathbf{0} & \\ & & 0 & & & \\ & & & 1 & & \\ & & & & 0 & \\ & \mathbf{0} & & & & \ddots & \\ & & & & & & 0 \end{pmatrix}$$

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Completeness relationship

If we sum over a complete set of states, like the eigenstates of a Hermitian operator, we obtain the (useful) resolution of identity

$$\sum_n |\psi_n\rangle\langle\psi_n| = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & \mathbf{0} & & \\ & & 1 & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & \mathbf{0} & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} = \hat{I}$$

$$\hat{I} = \sum_n |\psi_n\rangle\langle\psi_n|$$

$$|\psi\rangle = \sum_n \langle\psi_n|\psi\rangle\,|\psi_n\rangle = \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle = \left(\sum_n |\psi_n\rangle\langle\psi_n|\right)|\psi\rangle$$

Completeness relationship

If we sum over a complete set of states, like the eigenstates of a Hermitian operator, we obtain the (useful) resolution of identity

$$\sum_n |\psi_n\rangle\langle\psi_n| = \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & 0 & & \\ & & 1 & & & & \\ & & & 1 & & & \\ & & & & 1 & & \\ & 0 & & & & \ddots & \\ & & & & & & 1 \end{pmatrix} = \hat{I}$$

If the eigenvalues indexed by n range over a continuous set of values, the summation becomes an integration

$$\hat{I} = \int |\psi_n\rangle\langle\psi_n|\, dn$$

Generalization of the 3rd postulate

In any measurement of the observable A associated with operator $\hat{A}$, the only values that will ever be observed are the eigenvalues, which satisfy the eigenvalue equation

$$\hat{A}|\psi_n\rangle = a_n\,|\psi_n\rangle \qquad\qquad \langle\psi_p|\psi_n\rangle = \delta_{p,n}$$

The result of a measurement is one of the set of eigenvalues (a_n) of $\hat{A}$

The probability of measuring eigenvalue (a_n) is given by

$$\mathcal{P}(a_n) = |\langle\psi_n|\psi\rangle|^2$$

Non degenerate

Right after the measurement with result (a_n), the system is projected onto the vector subspace $|\psi_n\rangle$

This means that a second measurement performed immediately after will produce the same result (a_n)

Generalization of the 3rd postulate

In case of degenerate eigenvalues the dimension of the Hilbert space is

$$(a_n) = g_n \geq 2$$

$$\hat{A}\left|\psi_{n,r_n}\right\rangle = a_n\left|\psi_{n,r_n}\right\rangle \quad \text{with} \quad r_n = 1, \ldots, g_n$$

The result of a measurement is one of the set of eigenvalues (a_n) of $\hat{A}$

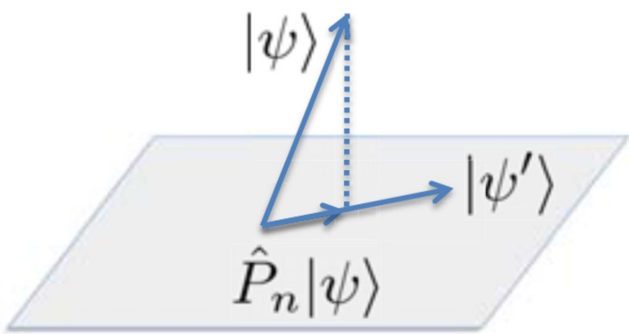
The probability of measuring eigenvalue (a_n) is given by

$$\mathcal{P}(a_n) = \sum_{r_n} |\langle\psi_{r_n}|\psi\rangle|^2$$

Degenerate

After the measurement

$$\frac{\hat{P}_n|\psi\rangle}{||\hat{P}_n|\psi\rangle||}$$



Infinite dimensional case

A "good operator": Hamiltonian of the harmonic oscillator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Discrete spectrum : $E_n = \hbar\omega\,(n + 1/2)$, $n \in \mathbb{N}$

Eigenfunctions (Hermite polynomials) $e^{-x^2/2a^2},\ x\,e^{-x^2/2a^2},\ \ldots\ a = \sqrt{\hbar / m\omega}$

Included in Hilbert space of square-integrable functions

A "delicate operator": the momentum

$$\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$$

Continuous spectrum $\hbar k$ → Set of real numbers

Eigenfunctions : e^{ikx}

Not included in Hilbert space of square-integrable functions

Position and momentum space

$$|\psi\rangle = \int dx\,|x\rangle\,\langle x|\psi\rangle = \int dp\,|p\rangle\,\langle p|\psi\rangle$$

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

is the value of the wave function at position x is simply the projection of the state $|\psi\rangle$ onto an eigenstate $|x\rangle$

$$|\,\langle x|\psi\rangle\,|^2$$

Probability of measurement of x

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

Probability amplitude for measurement of p

Inner product

$$\langle\phi|\psi\rangle = \langle\phi|(\int|x\rangle\,\langle x|\,dx)\psi\rangle = \int\langle\phi|x\rangle\,\langle x|\psi\rangle\,dx = \int\phi^*(x)\psi(x)dx$$

Position and momentum space

Conversion between $\psi(x)$ **and** $\psi(p)$:

$$\psi(p) = \langle p|\psi\rangle = \int \langle p|x\rangle \langle x|\psi\rangle \, dx$$
$$= \int e^{-ipx/\hbar}\psi(x)\frac{dx}{\sqrt{2\pi\hbar}}$$

Similarly $\psi(x) = \int e^{ipx/\hbar}\psi(p)\frac{dp}{\sqrt{2\pi\hbar}}.$

The conversion between position and momentum space is mathematically a Fourier transform because

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(ipx/\hbar).$$

Discrete vs continuous

$\hat{A}\,|a_n\rangle = a_n\,|a_n\rangle$ **with discrete eigenvalues** a_n

$\hat{B}\,|b_n\rangle = b_n\,|b_n\rangle$ **with continuous eigenvalues** b_n

Discrete	Continuous
$\langle a_m\|a_n\rangle = \delta_{mn}$	$\langle b_m\|b_n\rangle = \delta(b_m - b_n)$
$\sum_m \|a_m\rangle\langle a_m\| = 1$	$\int db_m\,\|b_m\rangle\langle b_m\| = 1$
$\|\alpha\rangle = \sum_m \|a_m\rangle\langle a_m\|\alpha\rangle$	$\|\beta\rangle = \int db_m\,\|b_m\rangle\langle b_m\|\beta\rangle$
$\sum_m \|\langle a_m\|\alpha\rangle\|^2 = 1$	$\int db_m \|\langle b_m\|\beta\rangle\|^2 = 1$
$\langle a_m\|A\|a_n\rangle = a_n\delta_{mn}$	$\langle b_m\|B\|b_n\rangle = b_n\delta(b_m - b_n)$

δ_{mn} **Kronecker delta function** $\delta(b_m - b_n)$ **Dirac delta function**

Commutators

Commutators between two operators are defined as

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

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

Heisenberg

Two operators commute (or are compatible) if $[\hat{A},\hat{B}] = 0$

To figure out commutation relations, apply the operators on a test function and look at the end result (sans test function)

Example: the canonical commutation relation $[\hat{x},\hat{p}] = i\hbar$

Note that if two operators commute, it becomes possible that the same state will be an eigenfunction of both operators. Then the two corresponding observables can be simultaneously specified for that state. The eigenvalues of the observables are basically “good quantum numbers” of the state

Commutators

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Example: the canonical commutation relation $[\hat{x}, \hat{p}] = i\hbar$

Generalization of the Heisenberg's uncertainty principle

$$\Delta a \Delta b \geq \frac{1}{2} \mid \langle \psi | [\hat{A}, \hat{B}] | \psi \rangle \mid$$

Time evolution

Evolution of the state vector $|\psi(t)\rangle$

$$i\hbar\frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle$$

If eigenstates of the Hamiltonian $\hat{H}$ are known (not time dependent)

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$$

We can write the following decomposition

$$|\psi(t)\rangle = \sum_n c_n(t)\,|\psi_n\rangle$$

$$|\psi(t)\rangle = \sum_n \langle\psi_n|\psi(t_0)\rangle\, e^{-i\frac{E_n(t-t_0)}{\hbar}}\,|\psi_n\rangle$$ with $$c_n(t_0) = \langle\psi_n|\psi(t_0)\rangle$$

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Propagator

$$|\psi(t)\rangle = \sum_n \langle\psi_n|\psi(t_0)\rangle \, e^{-i\frac{E_n(t-t_0)}{\hbar}} \, |\psi_n\rangle$$

$$|\psi(t)\rangle = \underbrace{\left(\sum_n e^{-i\frac{E_n(t-t_0)}{\hbar}} \, |\psi_n\rangle\langle\psi_n|\right)}_{\hat{U}(t-t_0)} |\psi(t_0)\rangle$$

$$\hat{U}(t,t_0) = \begin{pmatrix} e^{-i\frac{E_0(t-t_0)}{\hbar}} & 0 & 0 & \\ 0 & e^{-i\frac{E_1(t-t_0)}{\hbar}} & 0 & \vdots \\ 0 & 0 & e^{-i\frac{E_2(t-t_0)}{\hbar}} & \\ & \cdots & & \end{pmatrix}$$

Time evolution with propagator

In absence of any measurement the evolution of the state vector $|\psi(t)\rangle$ is given by

$$i\hbar\frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle$$

$$|\psi(t)\rangle = \hat{U}(t-t_0)\,|\psi(t_0)\rangle$$

The Hamiltonian generates the time evolution of the vector state

$\hat{U}(t-t_0)$ is a unitary operator such as $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$

with $$\hat{U}(t,t_0) = \exp\left(-i\frac{\hat{H}(t-t_0)}{\hbar}\right)$$

Summary

Wave Functions	Vectors	Dirac Notation
ψ	$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$	$\|\psi\rangle$
ψ^*	$\begin{pmatrix} b_1^* & b_2^* & \cdots & b_N^* \end{pmatrix}$	$\langle\psi\|$
$\psi(\vec{r})$	$\begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \end{pmatrix}$	$\langle r\|\psi\rangle$
$\int \psi^* \psi d\vec{r}$	$\begin{pmatrix} b_1^* & b_2^* & \cdots & b_N^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$	$\langle\psi\|\psi\rangle$
$\hat{A}\psi = \phi$	$[A] \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$	$\hat{A}\,\|\psi\rangle = \|\phi\rangle$

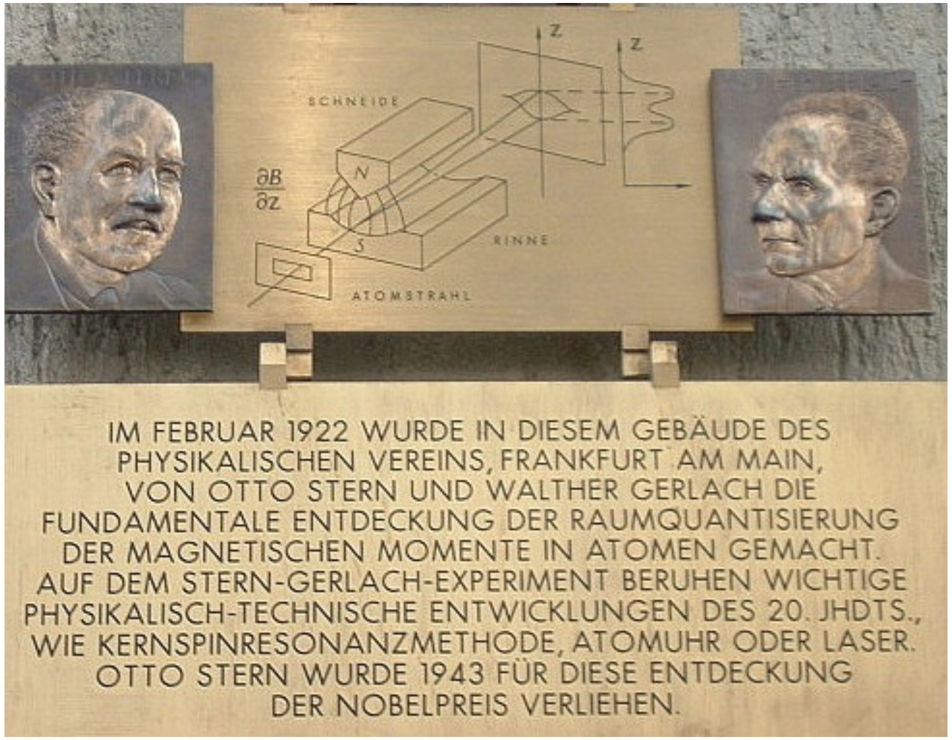
Summary

Wave Functions	Vectors	Dirac Notation
$\langle A \rangle = \int \psi^* \hat{A} \psi dr$	$\begin{pmatrix} b_1^* & b_2^* & \cdots & b_N^* \end{pmatrix} [A] \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$	$\langle \psi \vert A \vert \psi \rangle$
$\hat{A}\phi_n(x) = a_n \phi_n(x)$	$\begin{pmatrix} a_1 & 0 & & 0 \\ 0 & a_2 & & 0 \\ & & \ddots & \\ 0 & 0 & & a_N \end{pmatrix}$ in ϕ_n basis	$\hat{A} \vert \phi_n \rangle = a_n \vert \phi_n \rangle$
$\int \phi_m^* \phi_n d\vec{r} = \delta_{mn}$	$\begin{pmatrix} 0 & \cdots & 1 & \cdots & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \delta_{mn}$	$\langle \phi_m \vert \phi_n \rangle = \delta_{mn}$

Section 7

Spin angular momentum

The Stern-Gerlach experiment



1.
Principle and interpretation

The Stern and Gerlach experiment

1922: Stern and Gerlach (Silver atoms)

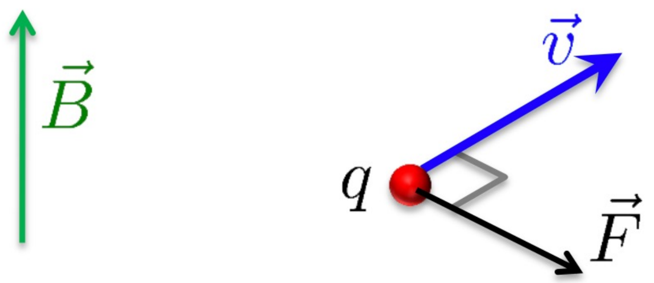
1927: Philips and Taylor (Hydrogen atoms)

The experiment demonstrated that the spatial orientation of angular momentum is quantized. In the original experiment, silver atoms were sent through a non-uniform magnetic field, which deflected them before being detected on a screen. The screen reveals discrete points of accumulation rather than a continuous distribution, owing to the quantum nature of spin

This experiment was decisive in convincing physicists of the reality of angular momentum quantization in all atomic-scale systems

Refreshers

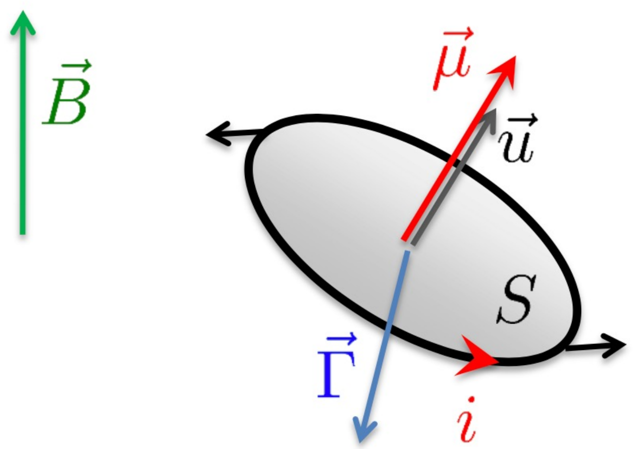
Charged particle



Lorentz's force

$$\vec{F} = q(\vec{v} \times \vec{B})$$

Magnetic dipole on a current loop



Magnetic moment

$$\vec{\mu} = iS\,\vec{u}$$

Torque

$$\vec{\Gamma} = \vec{\mu} \times \vec{B}$$

→ **rotation always in direction to align μ with B field**

Refreshers

Potential energy of interaction

$$W = -\vec{\mu}.\vec{B} = -\sum_{\alpha=x,y,z} \mu_\alpha B_\alpha$$

→ The magnetic moment of a compass is such that the corresponding potential energy is always minimized

Corresponding force

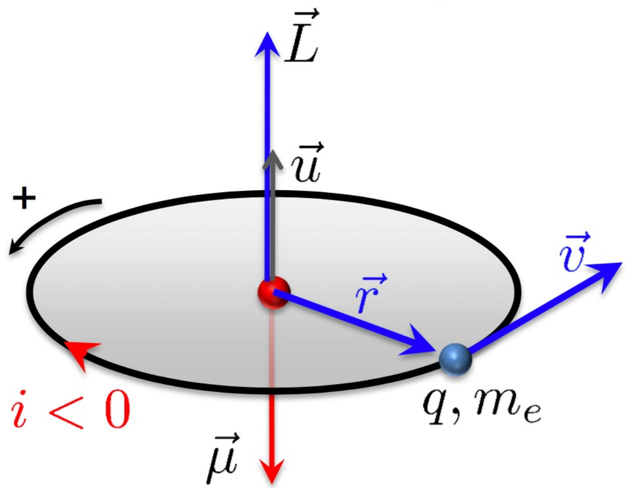
$$\vec{F} = -\vec{\nabla} W = \sum_{\alpha=x,y,z} \mu_\alpha \vec{\nabla} B_\alpha$$

Angular momentum of an electron in an atom (orbital motion)

$$\vec{L} = \vec{r} \times \vec{p}$$

Orbital angular momentum

Consider a semi-classical description of the hydrogen atom where electron (charge q<0, mass m) revolves in a circular orbit around the proton (uniform motion)



Orbital angular momentum

$$\vec{L} = \vec{r} \times \vec{p} = rmv\vec{u}$$

Magnetic moment $$\vec{\mu} = iS\,\vec{u} = \frac{qv}{2\pi r}\pi r^2 \vec{u} = \frac{qrv}{2}\vec{u}$$

$$\vec{\mu} = \gamma_0 \vec{L} \quad \textbf{with} \quad \gamma_0 = \frac{q}{2m}$$

Gyromagnetic ratio

The gyromagnetic ratio is negative for an electron

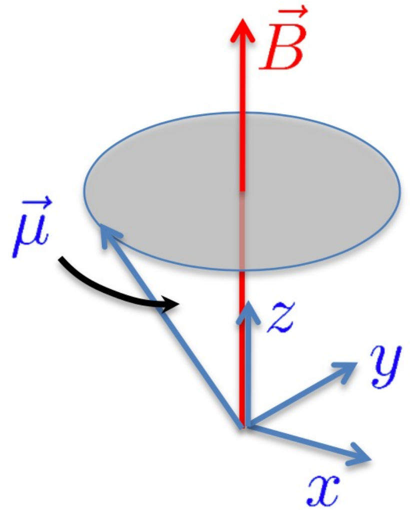
Larmor precession

Uniform magnetic field: $\vec{\Gamma} = \vec{\mu} \times \vec{B}$ **and** $\sum \vec{F} = \vec{0}$

Angular momentum theorem $\dfrac{d\vec{L}}{dt} = \vec{\Gamma} = \vec{\mu} \times \vec{B}$

$$\vec{\mu} = \gamma_0 \vec{L} \Rightarrow \frac{d\vec{\mu}}{dt} = \gamma_0 \vec{\mu} \times \vec{B} = -\gamma_0 \vec{B} \times \vec{\mu} = \vec{\omega}_0 \times \vec{\mu}$$

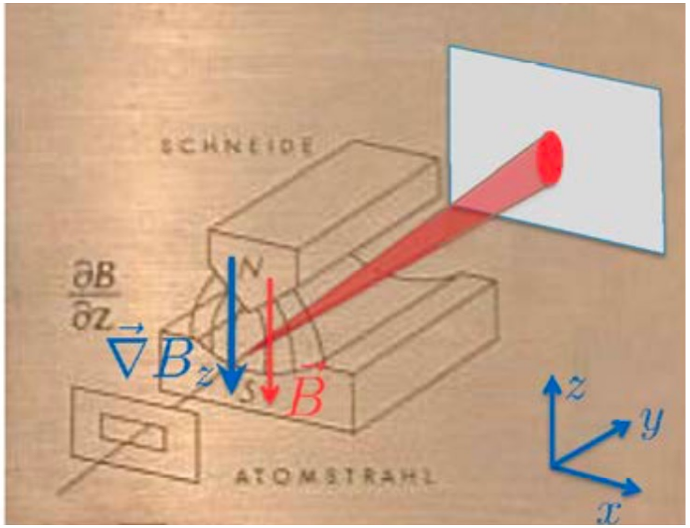
$\omega_0 = -\gamma_0 B$ **Larmor frequency**



$$\boxed{\begin{array}{ll} \dot{\mu}_x = -\omega_0 \mu_y & \mu_x(t) = \mu_\perp \cos(\omega_0 t + \varphi) \\ \dot{\mu}_y = +\omega_0 \mu_x & \mu_y(t) = \mu_\perp \sin(\omega_0 t + \varphi) \\ \dot{\mu}_z = 0 & W = -\mu_z B \quad \text{energy conservation} \end{array}}$$

The magnetic moment rotates about the magnetic field vector, describing a cone around the axis of the applied field

The Stern-Gerlach experiment



A beam of silver atoms is passed through an inhomogeneous magnetic field along z axis. This field would interact with the magnetic dipole of the atom and deflect it

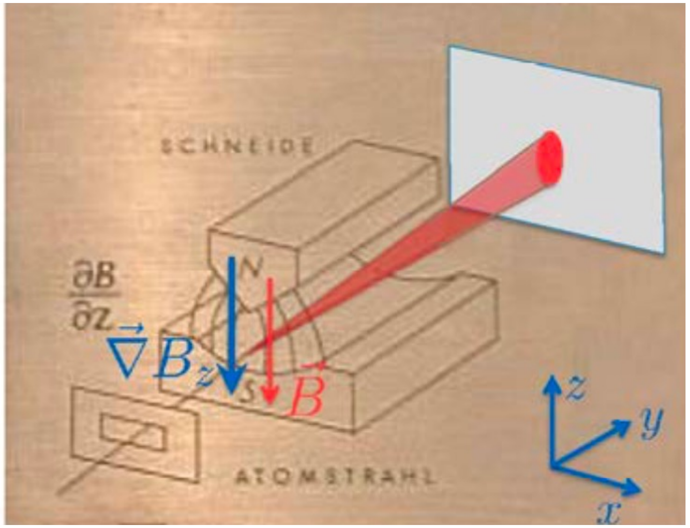
In classical physics, a continuous distribution, vertically orientated along z axis was expected due to the random orientation of the magnetic dipoles

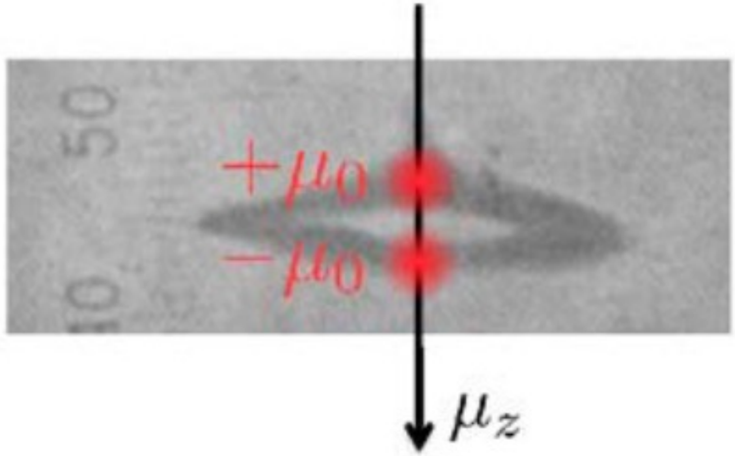
Larmor frequency $\frac{\omega_0}{2\pi} =$ 1 GHz with B = 0.1 T

$$< \mu_x > = < \mu_y > = 0$$

$$\vec{F} = -\vec{\nabla} W = \sum_{\alpha = x,y,z} \mu_\alpha \vec{\nabla} B_\alpha \approx \mu_z \vec{\nabla} B_z$$

The Stern-Gerlach experiment

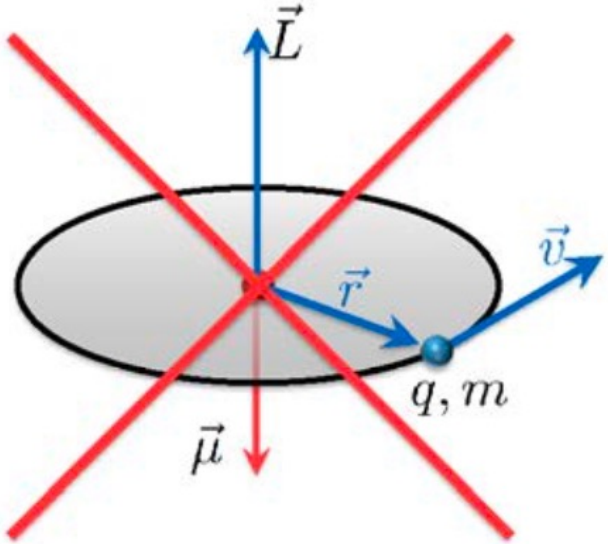




$$\mu_0 = \hbar \frac{q}{2m}$$

$$\mu_0 < 0$$

Wrong interpretation!



$$\vec{L} = \vec{r} \times \vec{p}$$

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Orbital angular momentum

The orbital state of the electron is described by its wavefunction $\psi(x, y, z)$

Owing to the invariance with respect to any rotation, the wavefunction of the ground state level is a radial function such that

$$\psi(x, y, z) = f(r) \qquad r = \sqrt{x^2 + y^2 + z^2}$$

1s orbital (Hydrogen atom)

$$\hat{L}_z \, |\psi\rangle = 0$$

The orbital angular momentum can not explain the result observed by Stern & Gerlach because the value of the orbital angular momentum is none for the ground state level which means that no deflection should be observed in the experiment

Spin- ½ particle

1924: Pauli postulated that the electron has a new quantum degree of freedom (or quantum number) with two possible values and with no classical equivalent

1925: Uhlenbeck and Goudsmit postulated the existence of a new intrinsic property of particles that behaved like an angular momentum

$$S_z = \pm\frac{\hbar}{2} \qquad \mu_z = 2\frac{q}{2m}S_z \qquad \gamma_e = \frac{q}{m}$$

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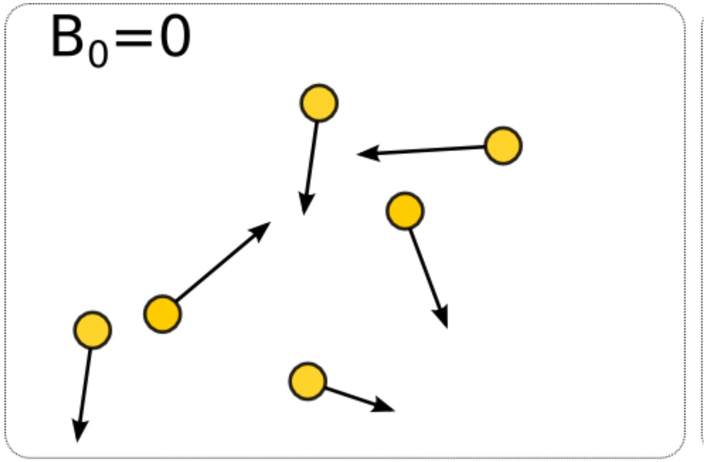
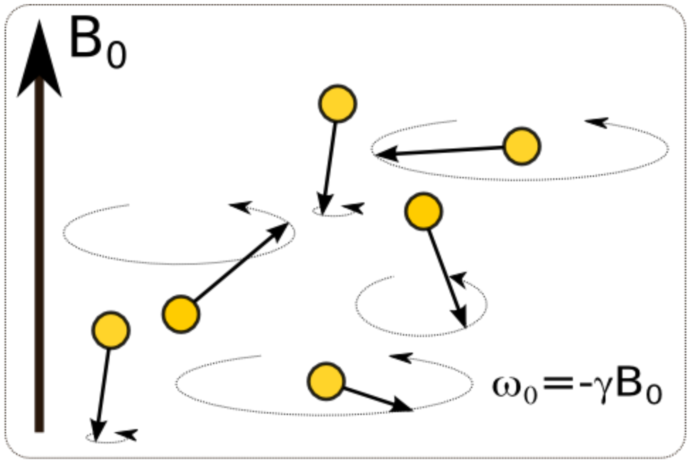
1924: Pauli postulated that the electron has a new quantum degree of freedom (or quantum number) with two possible values and with no classical equivalent

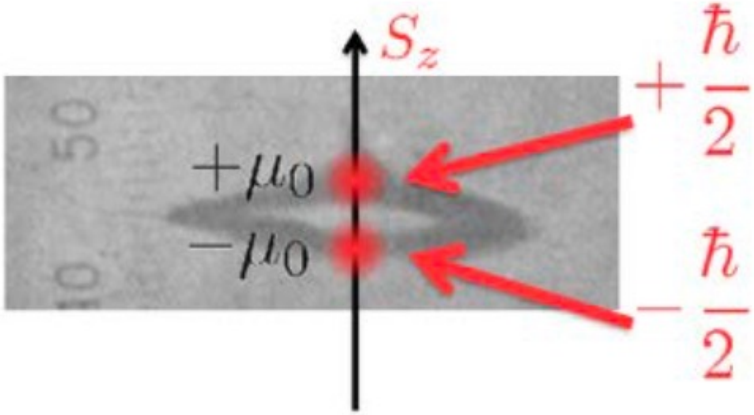
1925: Uhlenbeck and Goudsmit postulated the existence of a new intrinsic property of particles that behaved like an angular momentum

The existence of spin angular momentum is inferred from experiments, such as the Stern–Gerlach experiment, in which particles are observed to possess an angular momentum that cannot be accounted for the orbital angular momentum alone

Spin angular momentum







$$\mu_0 = \frac{\hbar}{2}\frac{q}{m}$$

Two possible results $S_z = \pm\frac{\hbar}{2}$

The Stern-Gerlach apparatus allows to measure the observable S_z that is the projection of the spin S along z axis

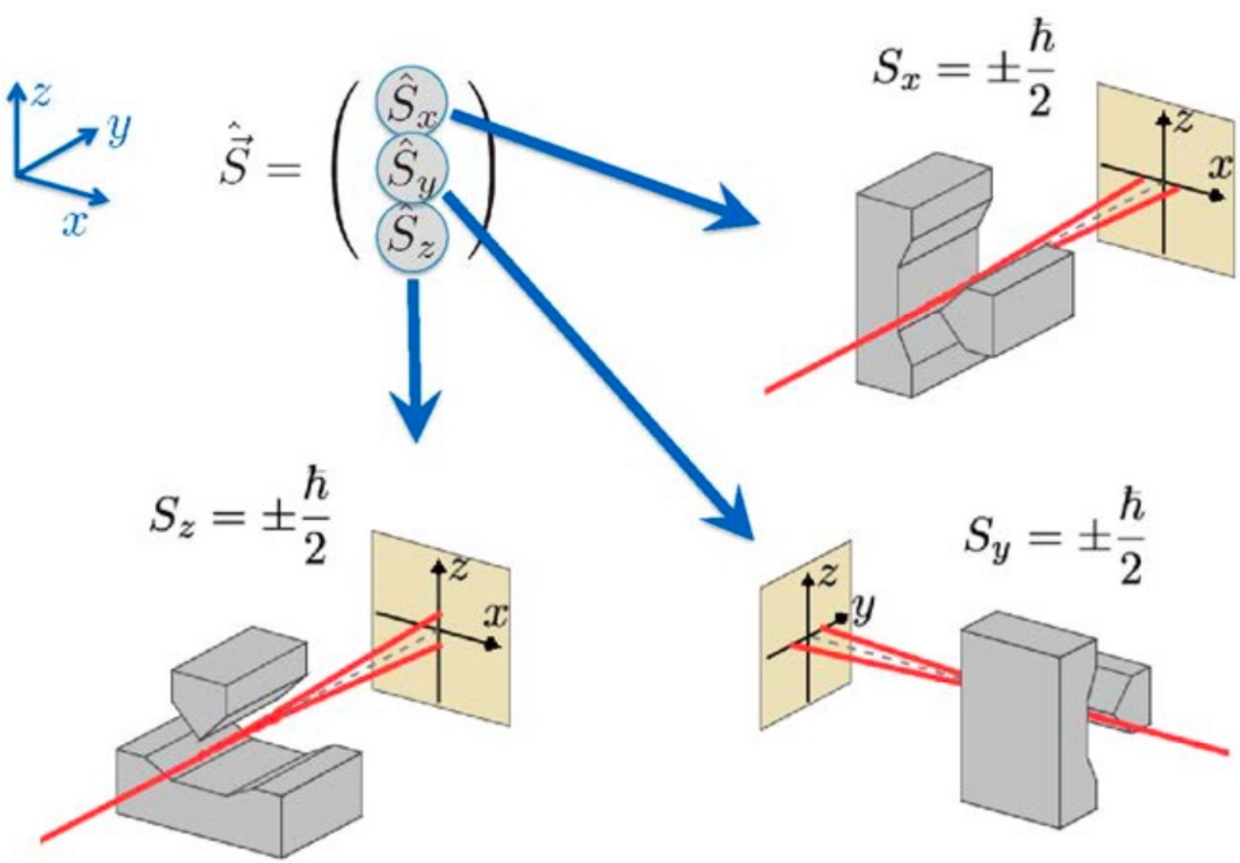
2.
Constructions of the Observables

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$$

$$[\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x$$

$$[\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y$$

Three components for the spin



In contrast to orbital angular momentum, the spin DOES NOT correspond to rotation around a geometric axis. It is an intrinsic property of quantum particles, but we will se that the effects are angular momentum-like

Construction of the operators

Hilbert's space describing the spin of the electron Ω_{spin}

Observable: $\hat{S}_z$ Eigenvalues: $\pm\frac{\hbar}{2}$ $\Rightarrow$ $\dim[\Omega_{spin}] \geq 2$

Minimalist assumption $\dim[\Omega_{spin}] = 2$

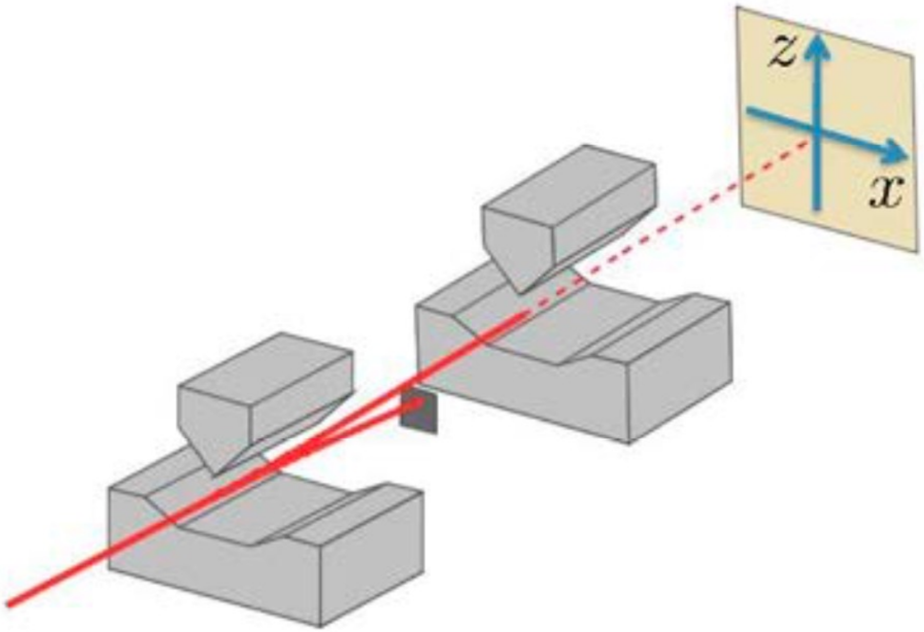
Consider $|+\rangle_z$ and $|-\rangle_z$ the eigenvectors of $\hat{S}_z$

$$\hat{S}_z |\pm\rangle_z = \pm\frac{\hbar}{2} |\pm\rangle_z$$

$\{|+\rangle_z, |-\rangle_z\}$ is a basis of Ω_{spin}

In this basis, $\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

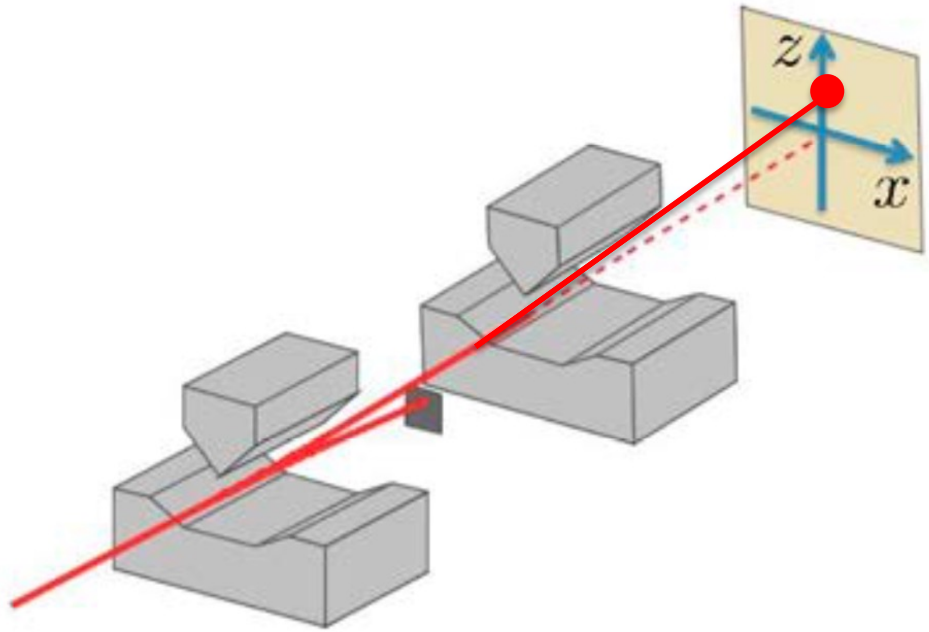
Quiz 5



What do you expect after the second Stern-Gerlach apparatus?

1. **One spot**
2. **Two spots**
3. **Does not make sense**
4. **I do not know**

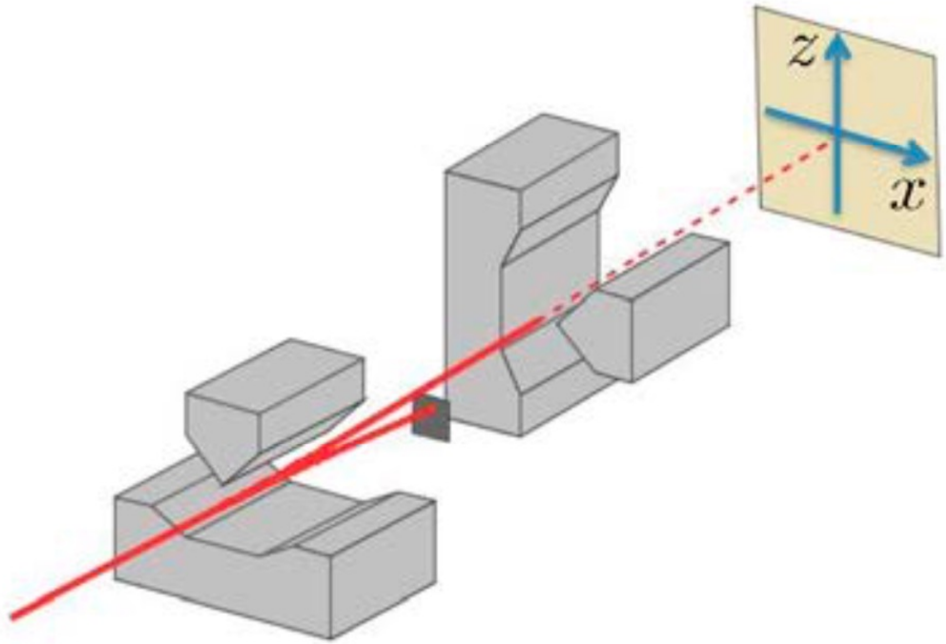
Quiz 5



What do you expect after the second Stern-Gerlach apparatus?

1. One spot
2. Two spots
3. Does not make sense
4. I do not know

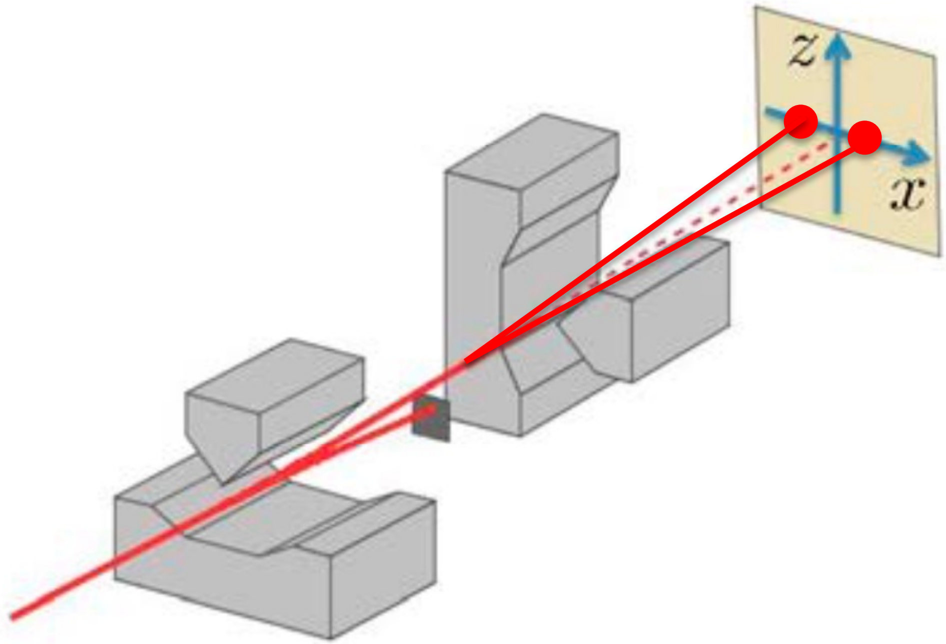
Quiz 6



What do you expect after the second Stern-Gerlach apparatus?

1. One spot at the center
2. Two spots shifted along z-axis
3. Two spots shifted along x-axis
4. I do not know

Quiz 6



What do you observe after the second Stern-Gerlach apparatus?

1. **One spot at the center**
2. **Two spots shifted along z-axis**
3. **Two spots shifted along x-axis**
4. **I do not know**

Construction of the operators

(1) $\hat{S}_x$ is an observable

In the basis $\{|+\rangle_z, |-\rangle_z\}$

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} \alpha_x & \beta_x^* \\ \beta_x & \gamma_x \end{pmatrix}$$

$\alpha_x, \gamma_x \in \mathbb{R}$

$\beta_x \in \mathbb{C}$

Construction of the operators

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$\beta_x \in \mathbb{C}$

(2) As for $\hat{S}_z$ the eigenvalues of $\hat{S}_x$ are: $\hat{S}_x |\pm\rangle_x = \pm\frac{\hbar}{2}|\pm\rangle_x$

$$\mathrm{Tr}\{\hat{S}_x\} = \frac{\hbar}{2}(\alpha_x + \gamma_x) = 0 \Longrightarrow \alpha_x + \gamma_x = 0$$

$$\det\{\hat{S}_x\} = \alpha_x\gamma_x - |\beta_x|^2 = -\frac{\hbar^2}{4} \Longrightarrow |\beta_x|^2 - \alpha_x\gamma_x - = 1$$

Construction of the operators

(1) $\hat{S}_x$ is an observable

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$$\det\left\{\hat{S}_x\right\} = \alpha_x\gamma_x - |\beta_x|^2 = -\frac{\hbar^2}{4} \quad \Rightarrow \quad |\beta_x|^2 - \alpha_x\gamma_x - = 1$$

(3) For the state $|+\rangle_z$ measurement of $\hat{S}_x$ produces two identical spots

$$< S_x >= \frac{1}{2}\left(\frac{\hbar}{2}\right) + \frac{1}{2}\left(\frac{-\hbar}{2}\right) = 0 \qquad {}_z\langle + | \hat{S}_x | + \rangle_z = \frac{\hbar}{2}\alpha_x = 0$$

$$\Rightarrow \quad \alpha_x = 0 \quad \gamma_x = 0 \quad |\beta_x| = 1$$

Construction of the operators

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & e^{-i\phi_x} \\ e^{i\phi_x} & 0 \end{pmatrix}$$

Consider the new basis $\left\{|+\rangle_z', |-\rangle_z'\right\}$ **with** $|\pm\rangle_z' = e^{\mp i\phi_x/2}\,|\pm\rangle_z$

$\langle\pm|_z' = \langle\pm|_z\, e^{\pm i\phi_x/2}$

$$\Rightarrow \quad {}_z'\langle -|\hat{S}_x|+\rangle_z' = {}_z\langle -|\hat{S}_x|+\rangle_z\, e^{-i\phi_x} = \frac{\hbar}{2}$$

In this new basis we have (for simplicity let us call it $\left\{|+\rangle_z, |-\rangle_z\right\}$ **)**

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

And, $\hat{S}_x\,|\pm\rangle_x = \pm\frac{\hbar}{2}\,|\pm\rangle_x \qquad |+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Construction of the operators

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & e^{-i\phi_y} \\ e^{i\phi_y} & 0 \end{pmatrix}$$

$${}_z\langle +|\hat{S}_y|+\rangle_z = 0$$

$${}_x\langle +|\hat{S}_y|+\rangle_x = 0$$

$${}_x\langle +|\hat{S}_y|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & e^{-i\phi_y} \\ e^{i\phi_y} & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$${}_x\langle +|\hat{S}_y|+\rangle_x = \frac{\hbar}{2}\cos\phi_y = 0 \quad \Rightarrow \quad \phi_y = \pm\frac{\pi}{2}$$

By convention and to match the experiments, we take: $\phi_y = +\frac{\pi}{2}$

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Pauli matrices

Pauli matrices for spin ½-particle

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with $\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$

Note that these three observables do not commute

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$$

$$[\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x$$

$$[\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y$$

Summary

Pauli matrices for electron spin description

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

with $\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$

Same commutations relationships than the orbital angular momentum

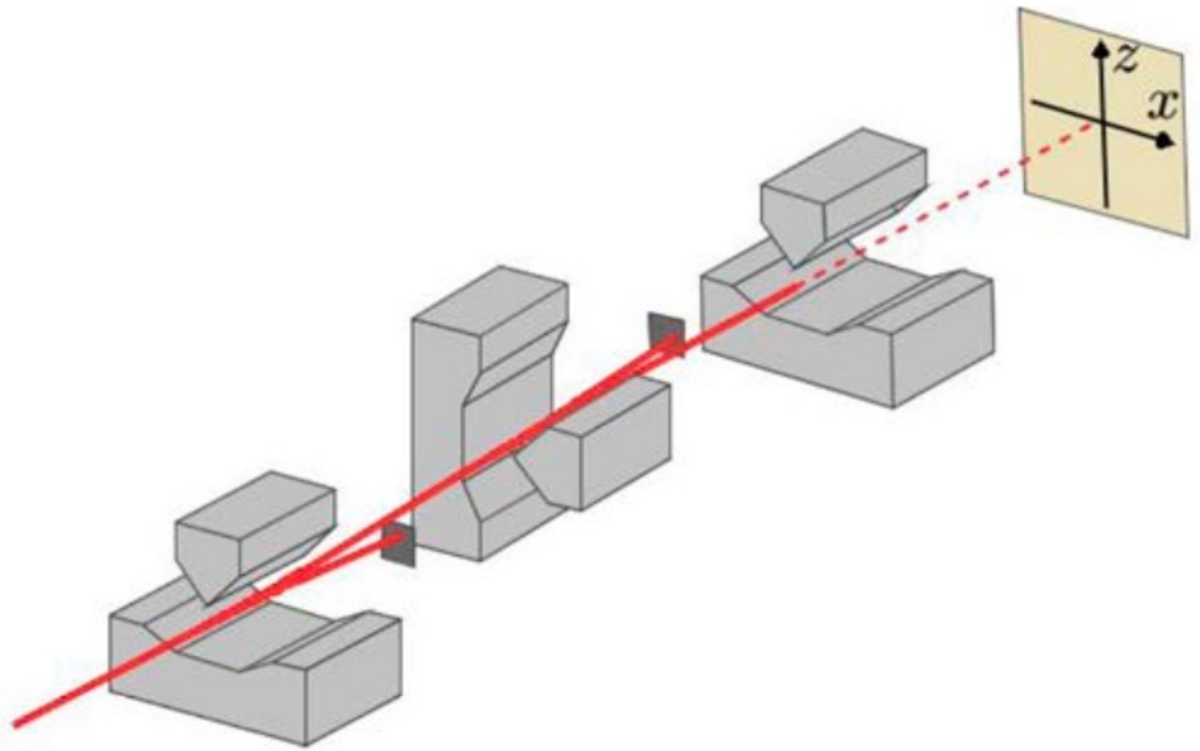
$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z \qquad [\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$$

$$[\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x \qquad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$$

$$[\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y \qquad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

→ The spin can indeed be seen an additional angular momentum

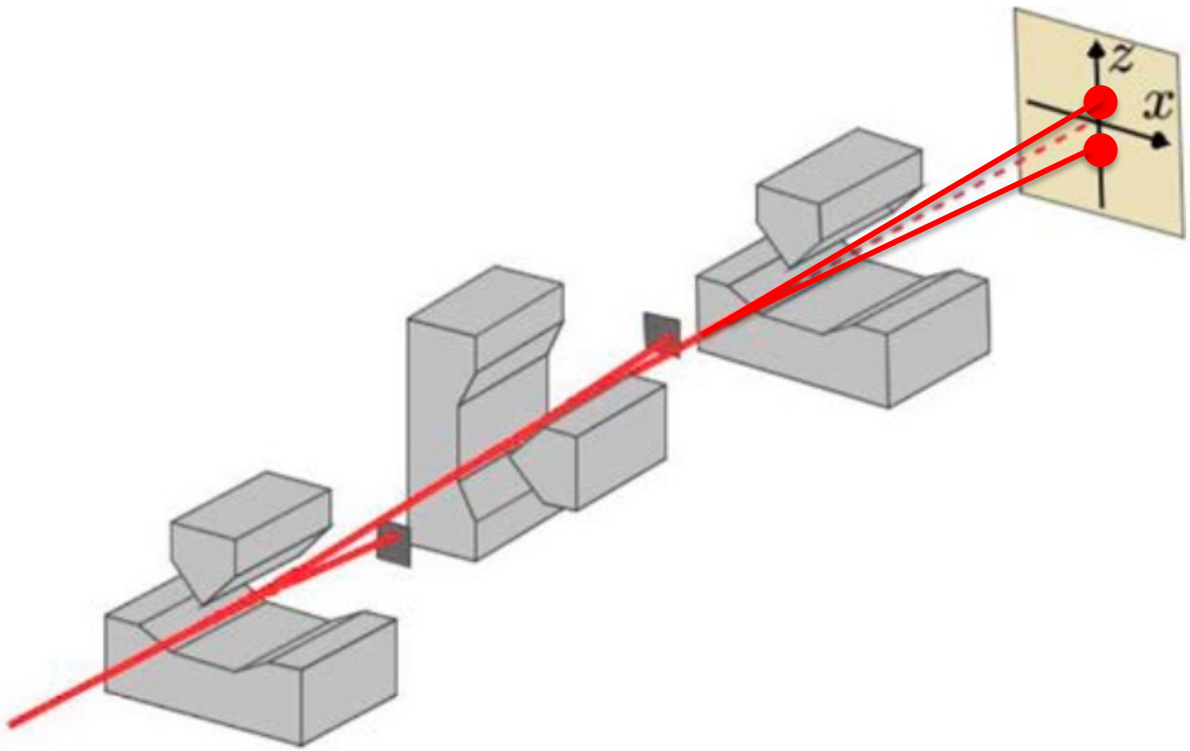
Quiz 7



What do you observe after the third Stern-Gerlach apparatus?

1. **One spot**
2. **Two spots**

Quiz 7

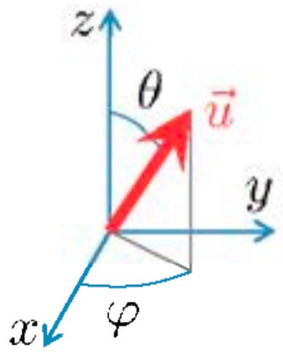


What do you observe after the third Stern-Gerlach apparatus?

1. **One spot**
2. **Two spots**

The observable $\hat{\vec{S}}.\vec{u}$

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



$$\vec{u} = \begin{Bmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{Bmatrix}$$

Spherical coordinates

$$\hat{\vec{S}}.\vec{u} = \hat{S}_x u_x + \hat{S}_y u_y + \hat{S}_z u_z$$

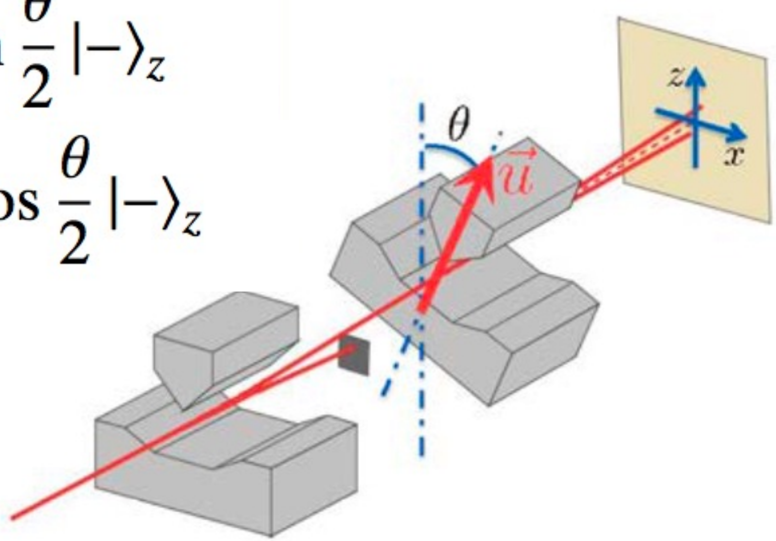
$$= \frac{\hbar}{2}\sin\theta\cos\varphi\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{\hbar}{2}\sin\theta\sin\varphi\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{\hbar}{2}\cos\theta\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{\vec{S}}.\vec{u} = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \qquad (\hat{S}.\vec{u})\,|\pm\rangle_{\vec{u}} = \pm\frac{\hbar}{2}\,|\pm\rangle_{\vec{u}}$$

The observable $\hat{\vec{S}}.\vec{u}$

$$|+\rangle_{\vec{u}} = e^{-i\varphi/2}\cos\frac{\theta}{2}|+\rangle_z + e^{i\varphi/2}\sin\frac{\theta}{2}|-\rangle_z$$

$$|-\rangle_{\vec{u}} = -e^{-i\varphi/2}\sin\frac{\theta}{2}|+\rangle_z + e^{i\varphi/2}\cos\frac{\theta}{2}|-\rangle_z$$



Measurement of

$$\hat{\vec{S}}.\vec{u} = \hat{S}_z\cos\theta + \hat{S}_x\sin\theta$$

for a system prepared in quantum state $|+\rangle_z$

Similar to Malus's law for light polarization but here for the spin

$$\left\{\begin{array}{l} P_\theta(+\hbar/2) = |_{\vec{u}}\langle +|+\rangle_z|^2 = \cos^2\left(\frac{\theta}{2}\right) \\ P_\theta(-\hbar/2) = |_{\vec{u}}\langle -|+\rangle_z|^2 = \sin^2\left(\frac{\theta}{2}\right) \end{array}\right.$$

3.
Towards a complete description of the Stern-Gerlach experiment

Tensor product of two Hilbert spaces

Consider a quantum system (a) represented by an Hilbert space $\mathcal{E}_a$ with basis $\{|\alpha_m\rangle\}$

Consider a quantum system (b) represented by an Hilbert space $\mathcal{E}_b$ with basis $\{|\beta_n\rangle\}$

If (a) is in state $|\alpha_m\rangle$ and (b) $|\beta_n\rangle$ then the state of the total quantum system is

$$|\alpha_m\rangle \otimes |\beta_n\rangle = |\alpha_m\rangle|\beta_n\rangle = |\alpha_m, \beta_n\rangle = |m, n\rangle$$

Tensor product

$$\langle\alpha_m| \otimes \langle\beta_n| = \langle\alpha_m|\langle\beta_n| = \langle\alpha_m, \beta_n| = \langle m, n|$$

Tensor product vector space $\mathcal{E}_a \otimes \mathcal{E}_b$

Tensor product of two Hilbert spaces

Consider a quantum system (a) represented by an Hilbert space $\mathcal{E}_a$ with basis $\{|\alpha_m\rangle\}$

Consider a quantum system (b) represented by an Hilbert space $\mathcal{E}_b$ with basis $\{|\beta_n\rangle\}$

General expression of the state $|\psi\rangle \in \mathcal{E}_a \otimes \mathcal{E}_b$

$$|\psi\rangle = \sum_{n,m} c_{n,m} |\alpha_m\rangle \otimes |\beta_m\rangle$$

Example: 2D quantum harmonic oscillator

$$\psi(x,y) = \sum_{m,n} c_{m,n} \varphi_m(x) \varphi_n(y) \qquad |\psi\rangle = \sum_{m,n} c_{m,n} |\varphi_m\rangle \otimes |\varphi_n\rangle$$

Tensor product of two operators

Consider an operator $\hat{A}$ acting on Hilbert space $\mathcal{E}_a$

Consider an operator $\hat{B}$ acting on Hilbert space $\mathcal{E}_b$

Tensor product $\hat{A} \otimes \hat{B}$ or $\hat{A}\hat{B}$

$$(\hat{A} \otimes \hat{B}) |\alpha_m\rangle |\beta_n\rangle = (\hat{A} |\alpha_m\rangle)(\hat{B} |\beta_n\rangle)$$

Back to the Stern-Gerlach experiment

$$\mathcal{E}_H = \mathcal{E}_{\text{ex}} \otimes \mathcal{E}_{\text{in}}$$ **with** $$\mathcal{E}_{\text{ex}} = \mathcal{L}^2(\mathbb{R}^3)$$

$$|\psi\rangle = \sum_{n,\sigma=\pm} c_{n,\sigma}|\varphi_n\rangle \otimes |\sigma\rangle_z$$

$|\varphi_n\rangle$ **basis of** $\mathcal{L}^2(\mathbb{R}^3)$

$$= \underbrace{\boxed{\sum_n c_{n,+}|\varphi_n\rangle}}_{a_+|\varphi_+\rangle} \otimes |+\rangle_z + \underbrace{\boxed{\sum_n c_{n,-}|\varphi_n\rangle}}_{a_-|\varphi_-\rangle} \otimes |-\rangle_z$$

$$|a_+|^2 + |a_-|^2 = 1$$

$$|\psi\rangle = a_+ |\varphi_+\rangle \otimes |+\rangle_z + a_- |\varphi_-\rangle \otimes |-\rangle_z$$

Linear superposition between
(a) a wavepacket $\varphi_+(\vec{r})$ associated to a magnetic state $|+\rangle_z$
and
(a) a wavepacket $\varphi_-(\vec{r})$ associated to a magnetic state $|-\rangle_z$

Time evolution

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} \otimes \hat{I}_{\mathrm{int}} - B_z(\hat{\vec{r}}) \otimes \hat{\mu}_z$$

Time evolution

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} \otimes \hat{I}_{\text{int}} - B_z(\hat{\vec{r}}) \otimes \hat{\mu}_z$$

$$\hat{H}|\varphi\rangle \otimes |\pm\rangle_z = \frac{\hat{p}^2}{2m}|\varphi\rangle \otimes |\pm\rangle_z - B_z(\hat{\vec{r}})|\varphi\rangle \otimes \hat{\mu}_z\,|\pm\rangle_z$$

Time evolution

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} \otimes \hat{I}_{\text{int}} - B_z(\hat{\vec{r}}) \otimes \hat{\mu}_z$$

$$\hat{H}|\varphi\rangle \otimes |\pm\rangle_z = \frac{\hat{p}^2}{2m}|\varphi\rangle \otimes |\pm\rangle_z - B_z(\hat{\vec{r}})|\varphi\rangle \otimes (\pm\mu_0)|\pm\rangle_z$$

$$= \left(\hat{H}_\pm|\varphi\rangle\right) \otimes |\pm\rangle_z$$

$$\hat{H}_\pm = \frac{\hat{p}^2}{2m} + V_\pm(\hat{\vec{r}})$$

$$V_\pm(\vec{r}) = \mp\mu_0 B_z(\vec{r})$$

Time evolution

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} \otimes \hat{I}_{\text{int}} - B_z(\hat{\vec{r}}) \otimes \hat{\mu}_z$$

$$\hat{H}|\varphi\rangle \otimes |\pm\rangle_z = \frac{\hat{p}^2}{2m}|\varphi\rangle \otimes |\pm\rangle_z - B_z(\hat{\vec{r}})|\varphi\rangle \otimes (\pm\mu_0)|\pm\rangle_z$$

$$= \left(\hat{H}_\pm|\varphi\rangle\right) \otimes |\pm\rangle_z$$

$$\hat{H}_\pm = \frac{\hat{p}^2}{2m} + V_\pm(\hat{\vec{r}}) \qquad V_\pm(\vec{r}) = \mp\mu_0 B_z(\vec{r})$$

$$\hat{U}(t,t_0) = \exp\left(-i\hat{H}(t-t_0)/\hbar\right)$$

$$\hat{U}(t,t_0)|\varphi\rangle \otimes |\pm\rangle_z = \left(\hat{U}_\pm(t,t_0)|\varphi\rangle\right) \otimes |\pm\rangle_z$$

with $\hat{U}_\pm(t,t_0) = \exp\left(-i\hat{H}_\pm(t-t_0)/\hbar\right)$

Entanglement

$$|\psi(t_0)\rangle = |\varphi(t_0)\rangle \otimes (a_+|+\rangle_z + a_-|-\rangle_z)$$

Consider the factorizable state (no correlation)

$$|\psi(t)\rangle = a_+\hat{U}(t,t_0)|\varphi(t_0)\rangle \otimes |+\rangle_z + a_-\hat{U}(t,t_0)|\varphi(t_0)\rangle \otimes |-\rangle_z$$

$$= a_+\hat{U}_+(t,t_0)|\varphi(t_0)\rangle \otimes |+\rangle_z + a_-\hat{U}_-(t,t_0)|\varphi(t_0)\rangle \otimes |-\rangle_z$$

Time-evolution of a wavepacket with $V_+(\vec{r})$

Time-evolution of a wavepacket with $V_-(\vec{r})$

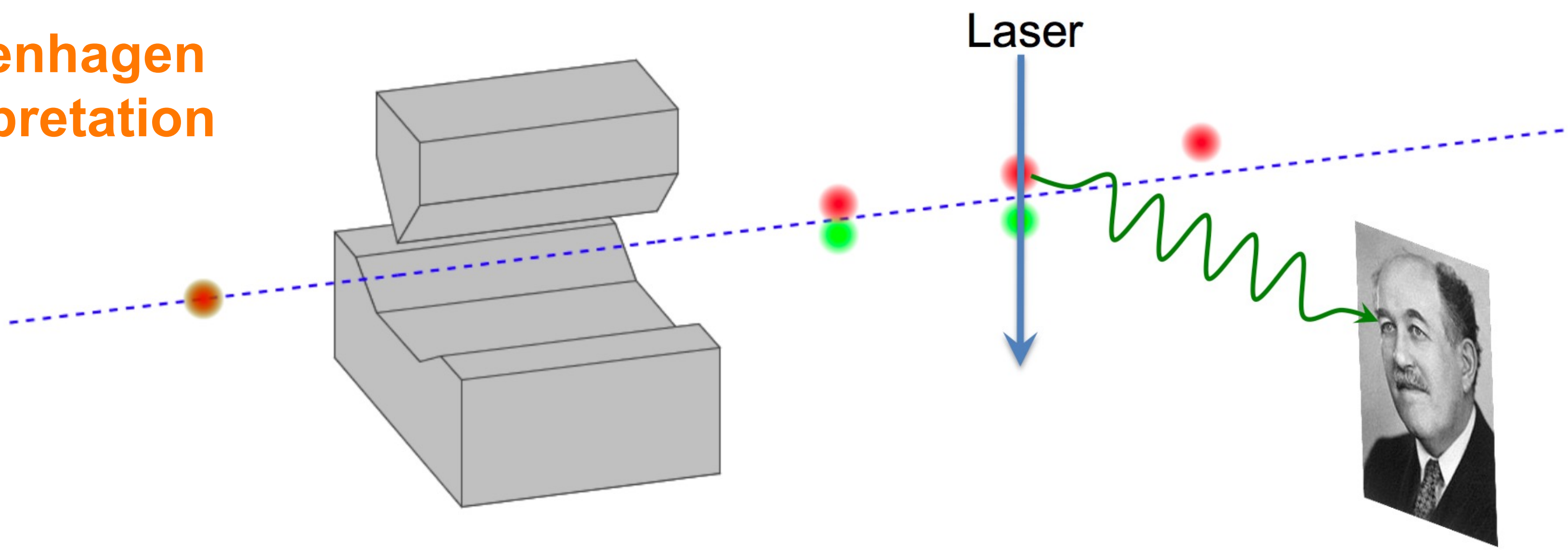
Entangled quantum state

$$|\psi\rangle = a_+\,|\varphi_+(t)\rangle \otimes |+\rangle_z + a_-\,|\varphi_-(t)\rangle \otimes |-\rangle_z$$

After the interaction with the Stern-Gerlach apparatus, there exists a direct correlation between the position of the atom and its magnetic state

Measurement in quantum mechanics

Copenhagen interpretation



$$|\psi(t_0)\rangle = a_+ \boxed{|\varphi(t_0)\rangle \otimes |+\rangle_z} + a_- \boxed{|\varphi(t_0)\rangle \otimes |-\rangle_z} \xrightarrow{\hat{U}(t,t_0)} |\psi(t)\rangle = a_+ \boxed{|\varphi_+(t)\rangle \otimes |+\rangle_z} + a_- \boxed{|\varphi_-(t)\rangle \otimes |-\rangle_z}$$

Measurement

$$|\varphi_+(t)\rangle \otimes |+\rangle_z$$

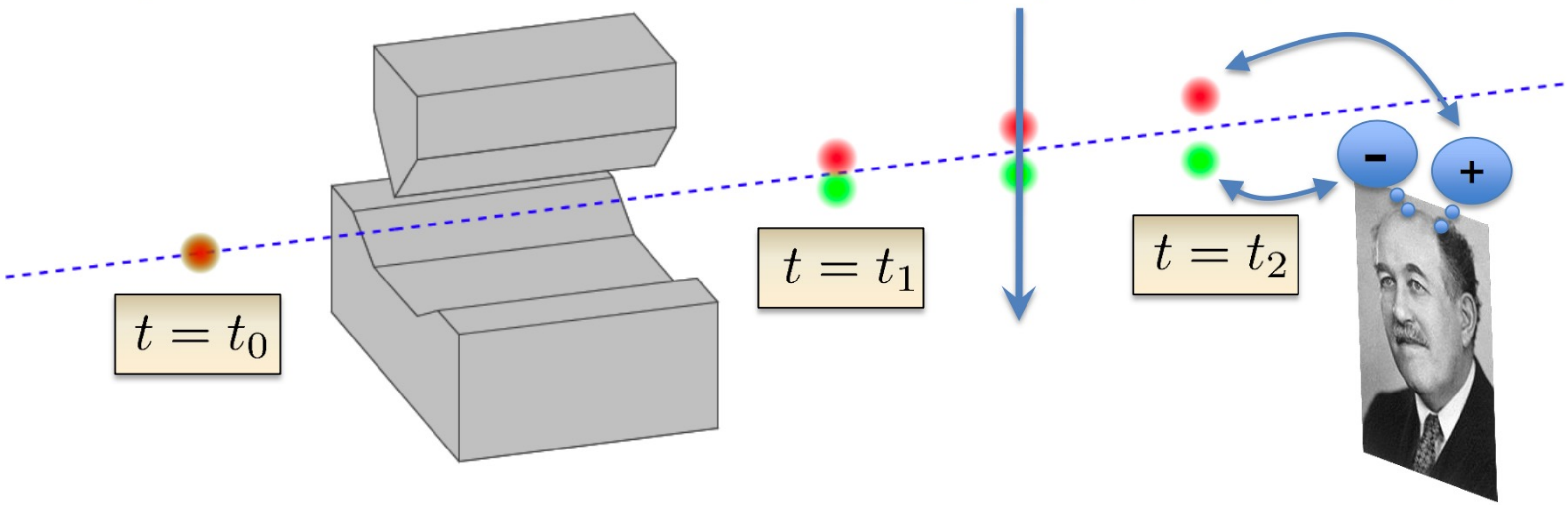
OR

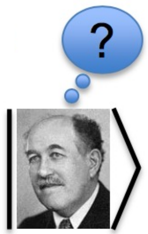
$$|\varphi_-(t)\rangle \otimes |-\rangle_z$$

Time-reversible **Time-irreversible**

Measuring the position gives a direct measurement of the spin

Many worlds interpretation of quantum mechanics

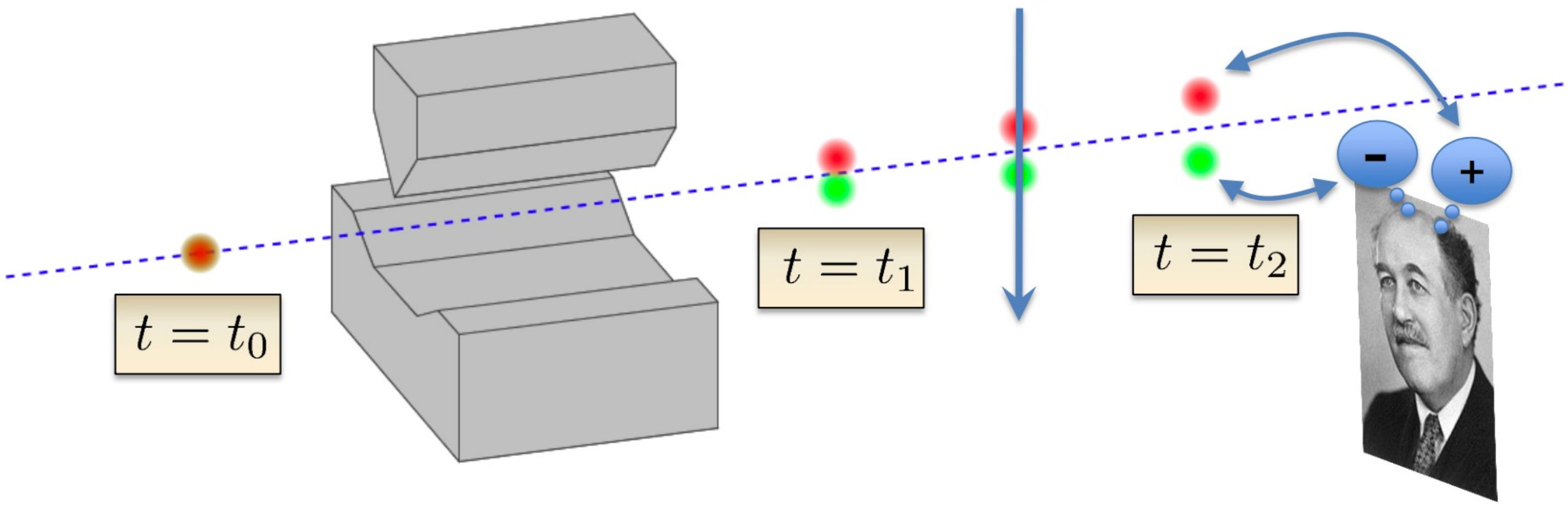


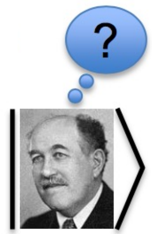
$t = t_0$ $\quad |\varphi(t_0)\rangle \otimes (a_+|+\rangle_z + a_-|-\rangle_z) \otimes$ 

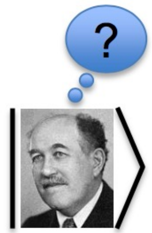
The observer is included into the description of the state vector

The 3rd postulate (measurement) is not invoked anymore

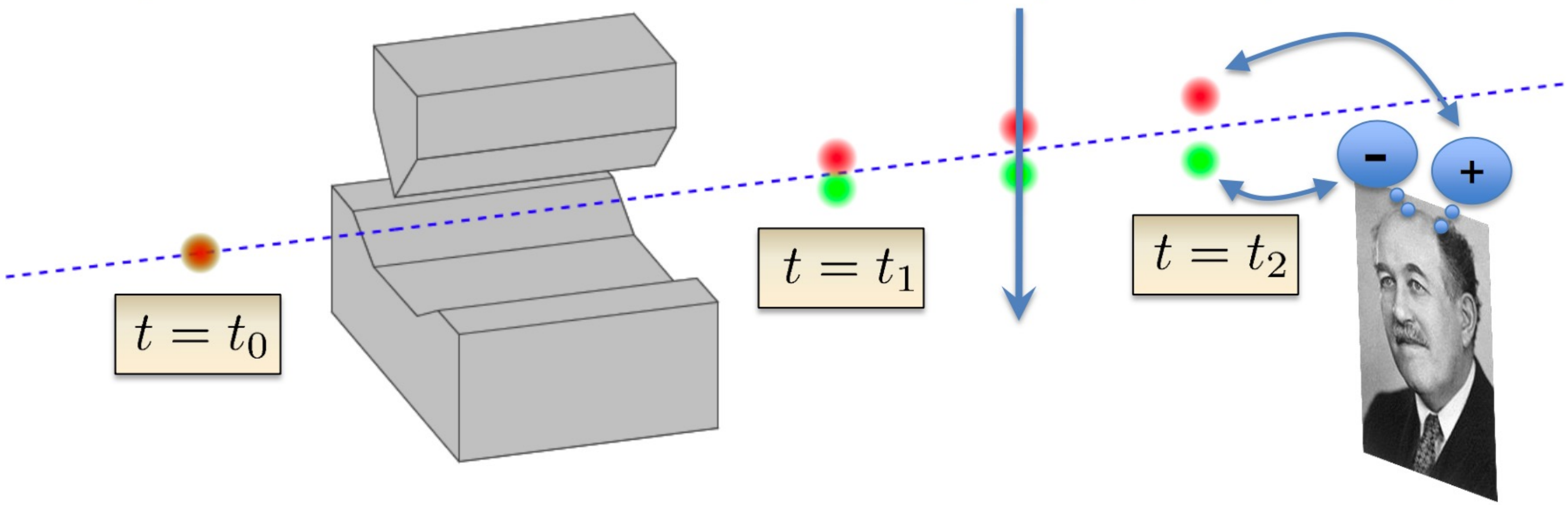
Many worlds interpretation of quantum mechanics

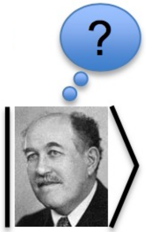


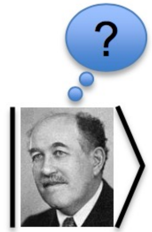
$t = t_0$ $\quad |\varphi(t_0)\rangle \otimes (a_+|+\rangle_z + a_-|-\rangle_z) \otimes$ 

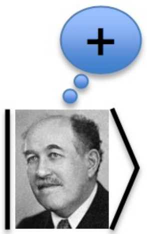
$t = t_1$ $\quad (a_+|\varphi_+(t_1)\rangle \otimes |+\rangle_z + a_-|\varphi_-(t_1)\rangle \otimes |-\rangle_z) \otimes$ 

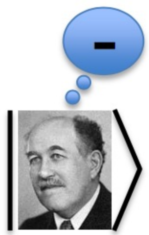
Many worlds interpretation of quantum mechanics



$t = t_0$ $\quad |\varphi(t_0)\rangle \otimes (a_+|+\rangle_z + a_-|-\rangle_z) \otimes$ 

$t = t_1$ $\quad (a_+|\varphi_+(t_1)\rangle \otimes |+\rangle_z + a_-|\varphi_-(t_1)\rangle \otimes |-\rangle_z) \otimes$ 

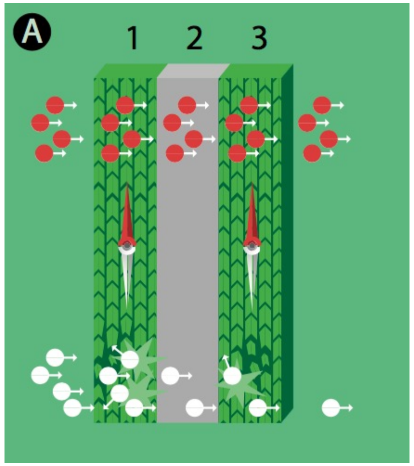
$t = t_2$ $\quad a_+|\varphi_+(t_2)\rangle \otimes |+\rangle_z \otimes$ 

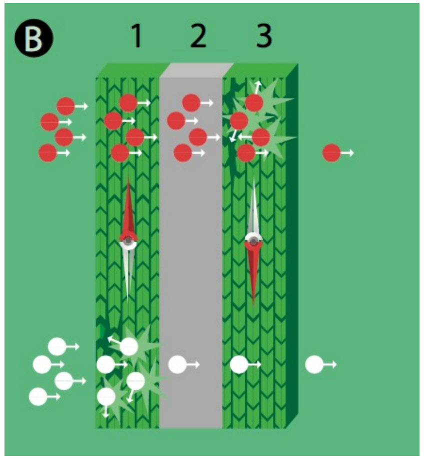
$+a_-|\varphi_-(t_2)\rangle \otimes |-\rangle_z \otimes$ 

Spintronic

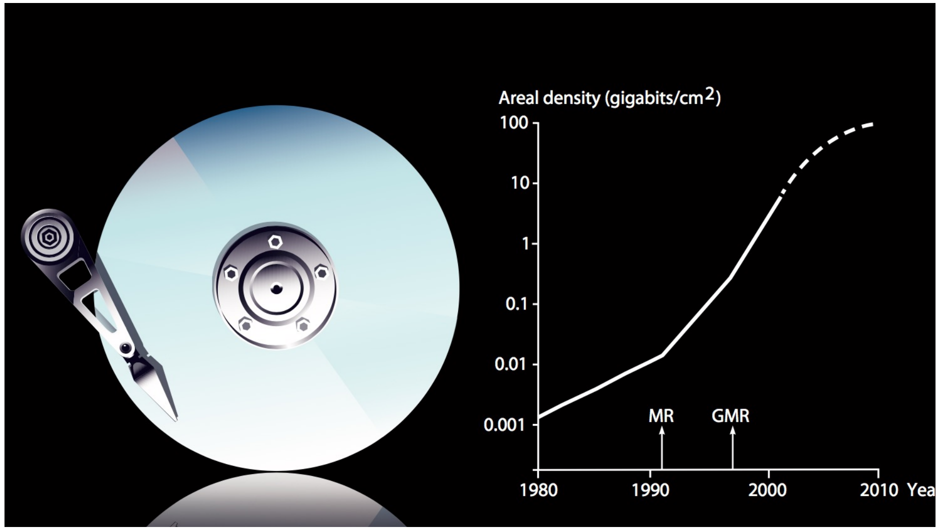
Giant Magneto Resistance (1988) involves small changes in magnetic fields creating major differences in electrical resistance

Albert Fert Peter Grünberg





Low resistance **High resistance**

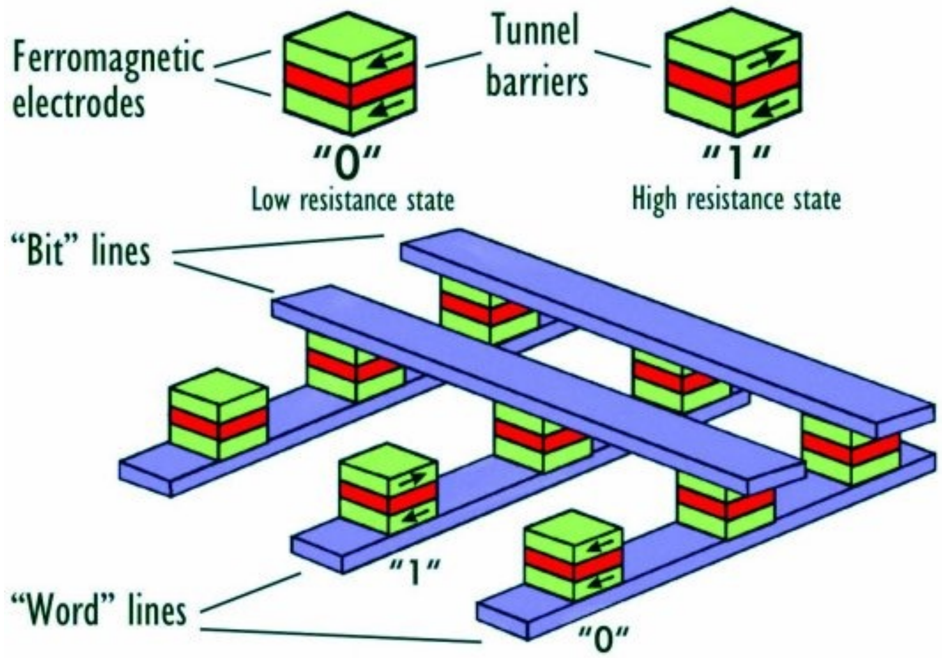


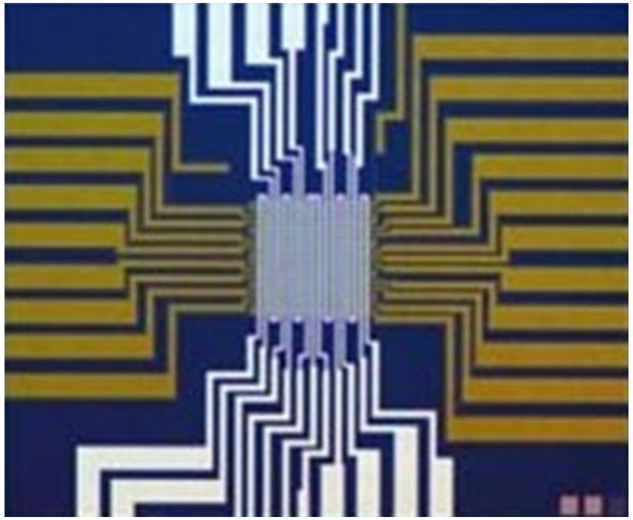
In a magnetic material, the scattering of electrons is driven by the direction of magnetization. The GMR arises because of the spin of the electron that induces a magnetic moment

→ Better read-out heads for pocket-size devices

Spintronic

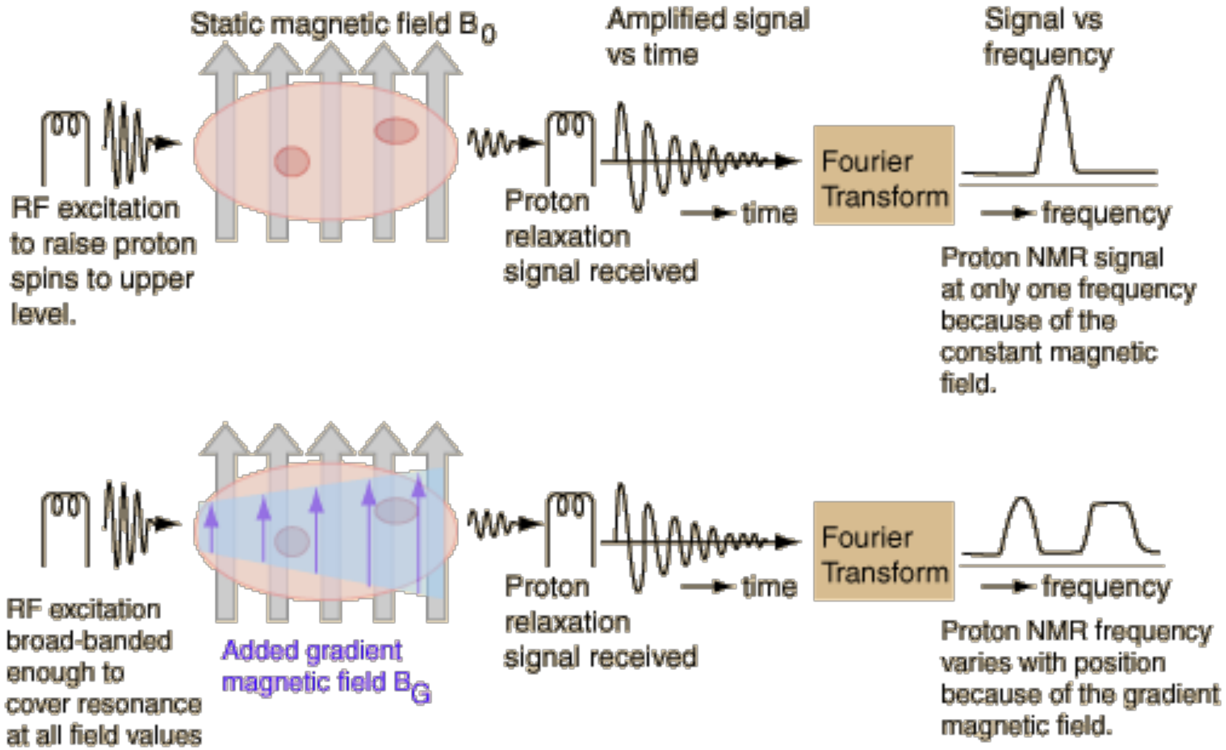
MRAM uses magnetic storage elements instead of electric used in conventional RAM





Tunnel junctions are used to read the information stored in Magnetoresistive Random Access Memory, typically a "0" for zero point magnetization state and "1" for antiparallel state

Nuclear magnetic resonance



1944

Isidor Isaac Rabi

1952

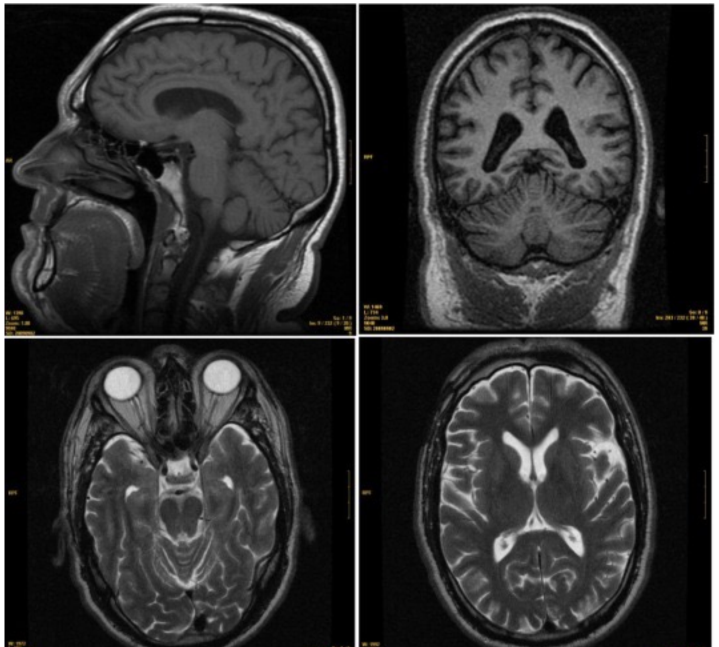
Felix Bloch

Edward Mills Purcell

A RF signal induces a transition between spin states. This "spin flip" places some of the spins in their higher energy state. If the RF signal is then switched off, the relaxation of the spins back to the lower state produces a RF signal at the resonant frequency associated with the spin flip

Nuclear magnetic resonance

Nuclear magnetic imaging

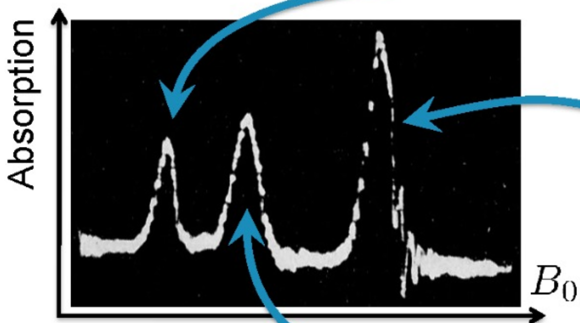


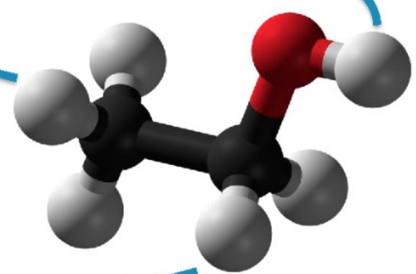
2003

Paul C. Lauterbur

Sir Peter Mansfield

Chemical spectroscopy
Spectrum of ethanol CH3-CH2-OH (1952)





Section 8

General description of the angular momentum

$$\hat{\vec{J}} = \left\{ \hat{J}_x, \hat{J}_y, \hat{J}_z \right\}$$

$$\hat{\vec{J}} \times \hat{\vec{J}} = i\hbar \hat{\vec{J}}$$

$$\left\{ \hat{J}^2, \hat{J}_z \right\}$$

1.
Orbital angular momentun

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

Orbital angular momentum

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \qquad \begin{cases} \hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{cases}$$

$$\begin{aligned} \left[\hat{L}_x, \hat{L}_y\right] &= [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \\ &= \hat{y}[\hat{p}_z, \hat{z}]\hat{p}_x + \hat{p}_y[\hat{z}, \hat{p}_z]\hat{x} \\ &= i\hbar\left(-\hat{y}\hat{p}_x + \hat{x}\hat{p}_y\right) = i\hbar\hat{L}_z \end{aligned}$$

$$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar\hat{L}_x \qquad \left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y \qquad \hat{\vec{L}} \times \hat{\vec{L}} = i\hbar\hat{\vec{L}}$$

It is not possible to simultaneously measure the different cartesian components of the orbital angular momentum operator

$\hat{L}^2$ operator

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$\left[\hat{L}_z, \hat{L}_x^2\right] = \left[\hat{L}_z, \hat{L}_x\right]\hat{L}_x + \hat{L}_x\left[\hat{L}_z, \hat{L}_x\right] = i\hbar\hat{L}_y\hat{L}_x + \hat{L}_x i\hbar\hat{L}_y$$

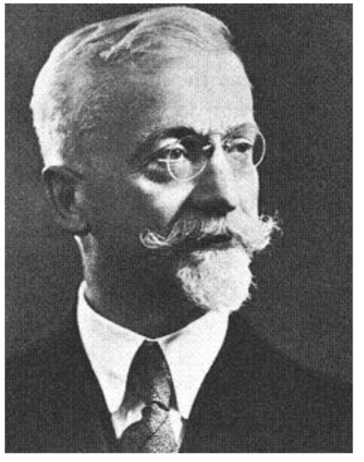
$$\left[\hat{L}_z, \hat{L}_y^2\right] = \left[\hat{L}_z, \hat{L}_y\right]\hat{L}_y + \hat{L}_y\left[\hat{L}_z, \hat{L}_y\right] = -i\hbar\hat{L}_x\hat{L}_y - \hat{L}_y i\hbar\hat{L}_x$$

$$\left[\hat{L}_z, \hat{L}_z^2\right] = 0$$

And we also have $\left[\hat{L}_x, \hat{L}^2\right] = 0$ $\quad \left[\hat{L}_y, \hat{L}^2\right] = 0$

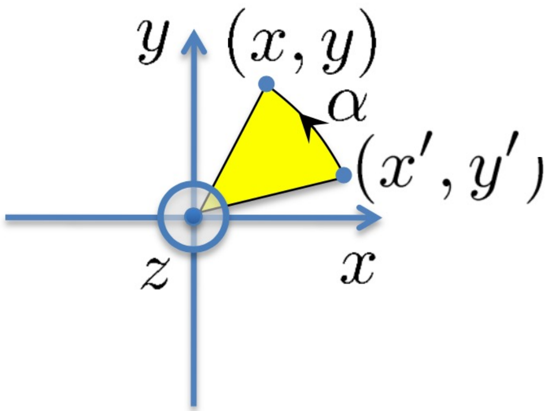
It is possible to simultaneously measure the norm of the components of the observable

2.
Algebraic theory of the angular momentum

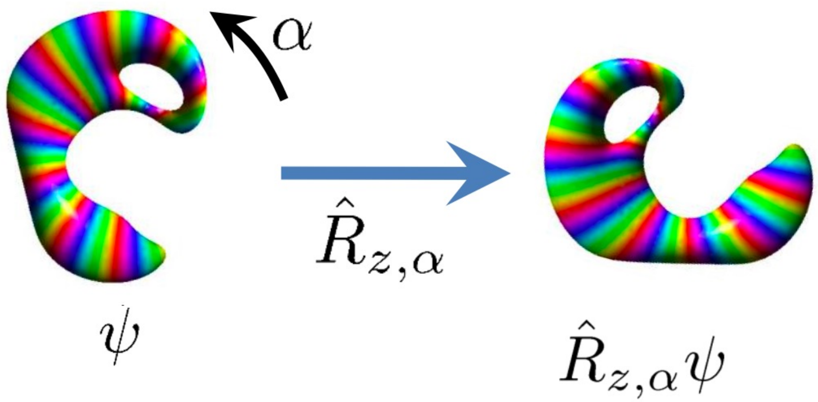


Elie Cartan
1869 - 1951

Representation of a rotation in Hilbert's space



Consider a rotation α around the z-axis on a wave function $\psi(x, y, z)$



$$\begin{cases} x' = x\cos\alpha + y\sin\alpha \\ y' = -x\sin\alpha + y\cos\alpha \\ z' = z \end{cases}$$

$$\begin{aligned} \left[\hat{R}_{z,\alpha}\psi\right](x, y, z) &= \psi(x', y', z') \\ &= \psi(x\cos\alpha + y\sin\alpha, -x\sin\alpha + y\cos\alpha, z) \end{aligned}$$

Representation of a rotation in Hilbert's space

Consider a rotation $\alpha \ll \pi$ around the z-axis

$$\left[\hat{R}_{z,\alpha}\psi\right](x,y,z) = \psi(x\cos\alpha + y\sin\alpha, -x\sin\alpha + y\cos\alpha, z)$$

$$\approx \psi(x + y\alpha, -x\alpha + y, z)$$

$$\approx \psi(x,y,z) - x\alpha\frac{\partial\psi}{\partial y} + y\alpha\frac{\partial\psi}{\partial x}$$

$$\approx \psi(x,y,z) - \alpha\frac{i}{\hbar}\left(x\hat{p}_y - y\hat{p}_x\right)\psi(x,y,z)$$

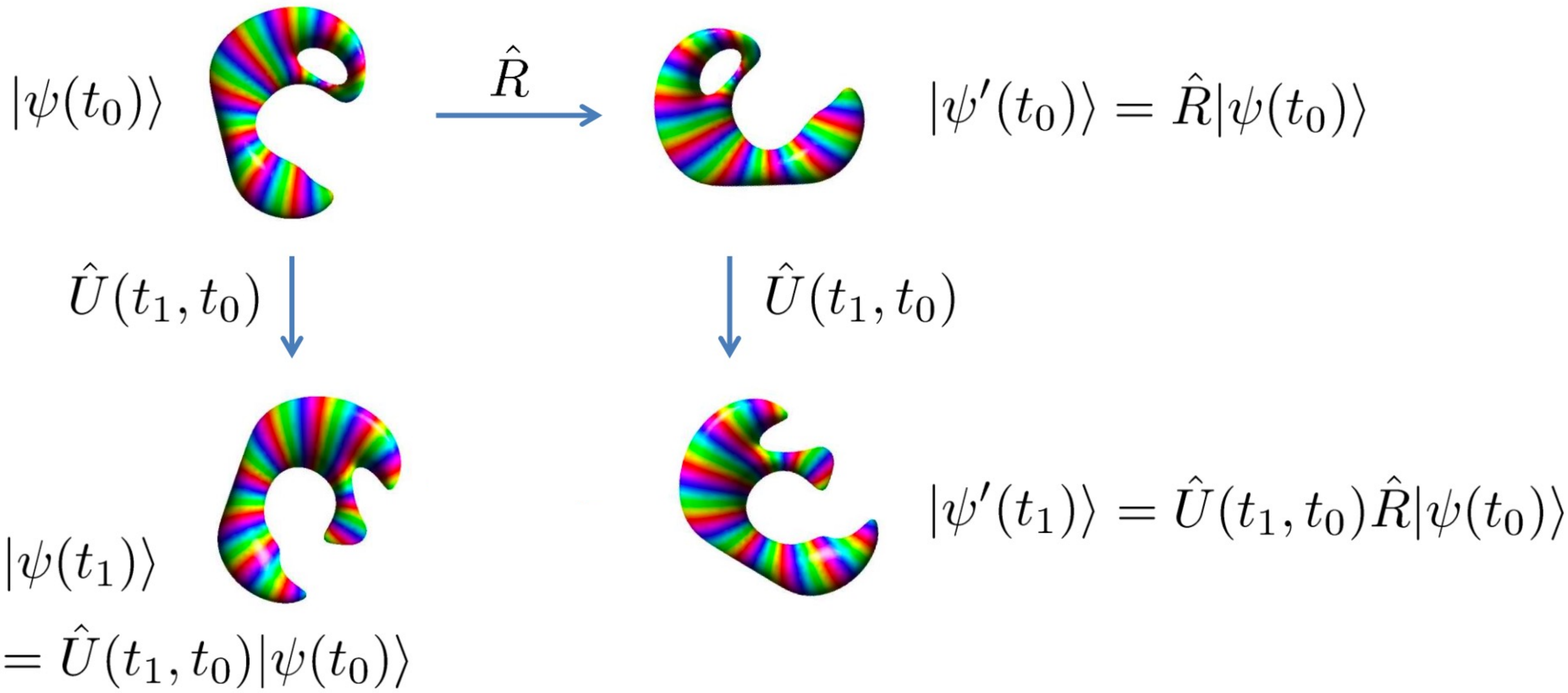
$$= \left(\hat{I} - \frac{i\alpha}{\hbar}\hat{L}_z\right)\psi(x,y,z)$$

$$\Rightarrow \quad \hat{R}_{z,\alpha} \approx \left(\hat{I} - \frac{i\alpha}{\hbar}\hat{L}_z\right)$$

$\hat{L}_x, \hat{L}_y, \hat{L}_z$ **are the infinitesimal generators of the rotation group**

Invariance and commutation

Consider the following system with a rotational invariance



Invariance and commutation

Consider the following system with a rotational invariance

$|\psi(t_0)\rangle$

$\xrightarrow{\hat{R}}$

$|\psi'(t_0)\rangle = \hat{R}|\psi(t_0)\rangle$

$\hat{U}(t_1, t_0) \downarrow$ $\qquad$ $\downarrow \hat{U}(t_1, t_0)$

$\xrightarrow{\hat{R}}$

$$|\psi(t_1)\rangle = \hat{U}(t_1, t_0)|\psi(t_0)\rangle$$

$$|\psi'(t_1)\rangle = \hat{U}(t_1, t_0)\hat{R}|\psi(t_0)\rangle = \hat{R}\hat{U}(t_1, t_0)|\psi(t_0)\rangle$$

$$\Rightarrow \left[\hat{R}, \hat{U}(t_1, t_0)\right] = 0$$

but $\psi(t + dt) = \psi(t) - \dfrac{idt}{\hbar}\hat{H}\psi(t)$

then $\hat{U}(t + dt, t) = \hat{I} - \dfrac{idt}{\hbar}\hat{H}$

$$\boxed{\left[\hat{R}, \hat{H}\right] = 0}$$

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Invariance and angular momentum

Rotational invariance $\hat{H}\hat{R}_{z,\alpha} = \hat{R}_{z,\alpha}\hat{H}$ **for any z and** $\underline{\alpha}$

This is true under small angle approximation

$$\hat{R}_{z,\alpha} \approx \left(\hat{I} - \frac{i\alpha}{\hbar}\hat{L}_z\right) \quad \Rightarrow \quad \hat{H}\hat{L}_z = \hat{L}_z\hat{H}$$

$$\boxed{\left[\hat{H},\hat{L}_x\right] = 0 \qquad \left[\hat{H},\hat{L}_y\right] = 0 \qquad \left[\hat{H},\hat{L}_z\right] = 0}$$

We can search a common basis to $\hat{H},\hat{L}^2$ **as well as to one of the cartesian coordinates of** $\hat{\vec{L}}$.

→ **We usually consider** $\left\{\hat{H},\hat{L}^2,\hat{L}_z\right\}$

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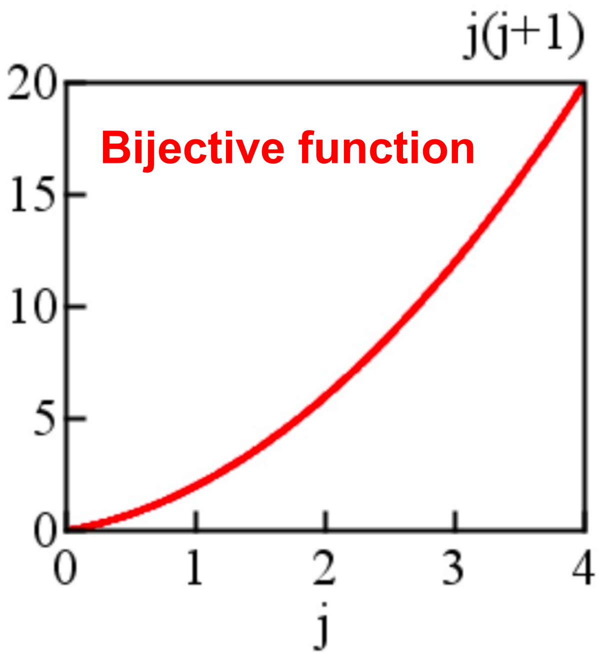
Eigenvalues of $\{\hat{J}^2, \hat{J}_z\}$

$$\langle\psi|\hat{J}^2|\psi\rangle = \sum_{\alpha=x,y,z} \langle\psi|\hat{J}_\alpha \hat{J}_\alpha|\psi\rangle = \sum_{\alpha=x,y,z} ||\hat{J}_\alpha|\psi\rangle||^2 \geq 0$$



Let us assume the following eigenvalues

$$\hat{J}^2 |\psi\rangle = j(j+1)\hbar^2 |\psi\rangle \qquad j \in \mathbf{R}^+$$

$$\hat{J}_z |\psi\rangle = m\hbar |\psi\rangle \qquad m \in \mathbf{R}$$

$\mathcal{E}_{j,m}$ **is the Hilbert space of J^2 and J_z with eigenvalues** $j(j+1)\hbar^2$ **and** $m\hbar$

Eigenvalues of $\left\{\hat{J}^2, \hat{J}_z\right\}$

The two observables $\left\{\hat{J}^2, \hat{J}_z\right\}$ share the same eigenstates

$$\hat{J}^2 |\psi\rangle = j(j+1)\hbar^2 |\psi\rangle$$

$$\hat{J}_z |\psi\rangle = m\hbar |\psi\rangle$$

j is called angular momentum quantum number. It must be integer or half-integer j = 0, 1/2, 1, 3/2, 2, etc.

For a given value of j, m that is called the magnetic quantum number can only take on integer values between -j and +j i.e., m = -j, -j+1,…, j-1, j

Only discrete values of angular momentum j are allowed

Let us prove this by using the algebraic theory developed by E. Cartan

Operators J_+ and J_-

Consider the following operators (see the quantum harmonic oscillator)

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \qquad (\hat{J}_+)^\dagger = \hat{J}_-$$

Not an observable

We also know the commutation relations

$$[\hat{J}^2, \hat{J}_\pm] = 0 \quad \text{and} \quad [\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm$$

$$\hat{J}_-\hat{J}_+ = (\hat{J}_x - i\hat{J}_y)(\hat{J}_x + i\hat{J}_y) = \hat{J}_x^2 + \hat{J}_y^2 + i[\hat{J}_x, \hat{J}_y]$$

$$\hat{J}_-\hat{J}_+ = \hat{J}_x^2 + \hat{J}_y^2 - \hbar\hat{J}_z$$

$$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_z(\hat{J}_z + \hbar\hat{I})$$

We can also demonstrate

$$\hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}_z(\hat{J}_z - \hbar\hat{I})$$

Action of J_+ and J_-

$$|\psi\rangle \in \mathcal{E}_{j,m} \qquad \hat{J}_{\pm}|\psi\rangle \quad ?$$

$$\hat{J}^2\hat{J}_+|\psi\rangle = \hat{J}_+\hat{J}^2|\psi\rangle = j(j+1)\hbar^2\hat{J}_+|\psi\rangle$$

Action of J_+ and J_-

$$|\psi\rangle \in \mathcal{E}_{j,m} \qquad\qquad \hat{J}_\pm |\psi\rangle \quad \textbf{?}$$

$$\hat{J}^2 \hat{J}_+ |\psi\rangle = \hat{J}_+ \hat{J}^2 |\psi\rangle = j(j+1)\hbar^2 \hat{J}_+ |\psi\rangle$$

$$\hat{J}_z \hat{J}_+ |\psi\rangle = (\hat{J}_+ \hat{J}_z + [\hat{J}_z, \hat{J}_+]) |\psi\rangle$$

$$\hat{J}_z \hat{J}_+ |\psi\rangle = (m\hbar \hat{J}_+ + \hbar \hat{J}_+) |\psi\rangle$$

$$\hat{J}_z \hat{J}_+ |\psi\rangle = (m+1)\hbar \hat{J}_+ |\psi\rangle$$

$\Rightarrow$ $\hat{J}_+ |\psi\rangle \in \mathcal{E}_{j,m+1}$ **or** $\hat{J}_+ |\psi\rangle = 0$

Action of J_+ and J_-

$$\boxed{|\psi\rangle \in \mathcal{E}_{j,m} \qquad\qquad \hat{J}_{\pm}|\psi\rangle \quad ?}$$

$$\hat{J}^2\hat{J}_-|\psi\rangle = \hat{J}_-\hat{J}^2|\psi\rangle = j(j+1)\hbar^2\hat{J}_-|\psi\rangle$$

Action of J_+ and J_-

$$|\psi\rangle \in \mathcal{E}_{j,m} \qquad \hat{J}_{\pm}|\psi\rangle \quad ?$$

$$\hat{J}^2 \hat{J}_- |\psi\rangle = \hat{J}_- \hat{J}^2 |\psi\rangle = j(j+1)\hbar^2 \hat{J}_- |\psi\rangle$$

$$\hat{J}_z \hat{J}_- |\psi\rangle = (\hat{J}_- \hat{J}_z + [\hat{J}_z, \hat{J}_-])|\psi\rangle$$

$$\hat{J}_z \hat{J}_- |\psi\rangle = (m\hbar \hat{J}_- - \hbar \hat{J}_-)|\psi\rangle$$

$$\hat{J}_z \hat{J}_- |\psi\rangle = (m-1)\hbar \hat{J}_- |\psi\rangle$$

$\Rightarrow$ $\hat{J}_- |\psi\rangle \in \mathcal{E}_{j,\, m-1}$ **or** $\hat{J}_- |\psi\rangle = 0$

Norm of $\hat{J}_\pm |\psi\rangle$

$|\psi\rangle \in \mathcal{E}_{j,m}$ **with** $\langle\psi|\psi\rangle = 1$

$$\| \hat{J}_+ |\psi\rangle \|^2 = \langle\psi|\hat{J}_-\hat{J}_+|\psi\rangle$$

$$\| \hat{J}_+ |\psi\rangle \|^2 = \langle\psi|\hat{J}^2 - \hat{J}_z(\hat{J}_z + \hbar\hat{I})|\psi\rangle$$

$$\| \hat{J}_+ |\psi\rangle \|^2 = [j(j+1) - m(m+1)]\hbar^2$$

Norm of $\hat{J}_{\pm}|\psi\rangle$

$|\psi\rangle \in \mathcal{E}_{j,m}$ **with** $\langle\psi|\psi\rangle = 1$

$$\| \hat{J}_+ |\psi\rangle \|^2 = \langle\psi|\hat{J}_-\hat{J}_+|\psi\rangle$$

$$\| \hat{J}_+ |\psi\rangle \|^2 = \langle\psi|\hat{J}^2 - \hat{J}_z(\hat{J}_z + \hbar\hat{I})|\psi\rangle$$

$$\| \hat{J}_+ |\psi\rangle \|^2 = [j(j+1) - m(m+1)]\hbar^2$$

$$\| \hat{J}_- |\psi\rangle \|^2 = \langle\psi|\hat{J}_+\hat{J}_-|\psi\rangle$$

$$\| \hat{J}_- |\psi\rangle \|^2 = \langle\psi|\hat{J}^2 - \hat{J}_z(\hat{J}_z - \hbar\hat{I})|\psi\rangle$$

$$\| \hat{J}_- |\psi\rangle \|^2 = [j(j+1) - m(m-1)]\hbar^2$$

What values for m and j?

$$||\hat{J}_{\pm}|\psi\rangle||^2 \geq 0 \Rightarrow m(m \pm 1) \leq j(j+1) \qquad \Rightarrow -j-1 \leq m \leq j$$

$$\Rightarrow -j \leq m \leq j+1$$

$$\Rightarrow \quad -j \leq m \leq j$$

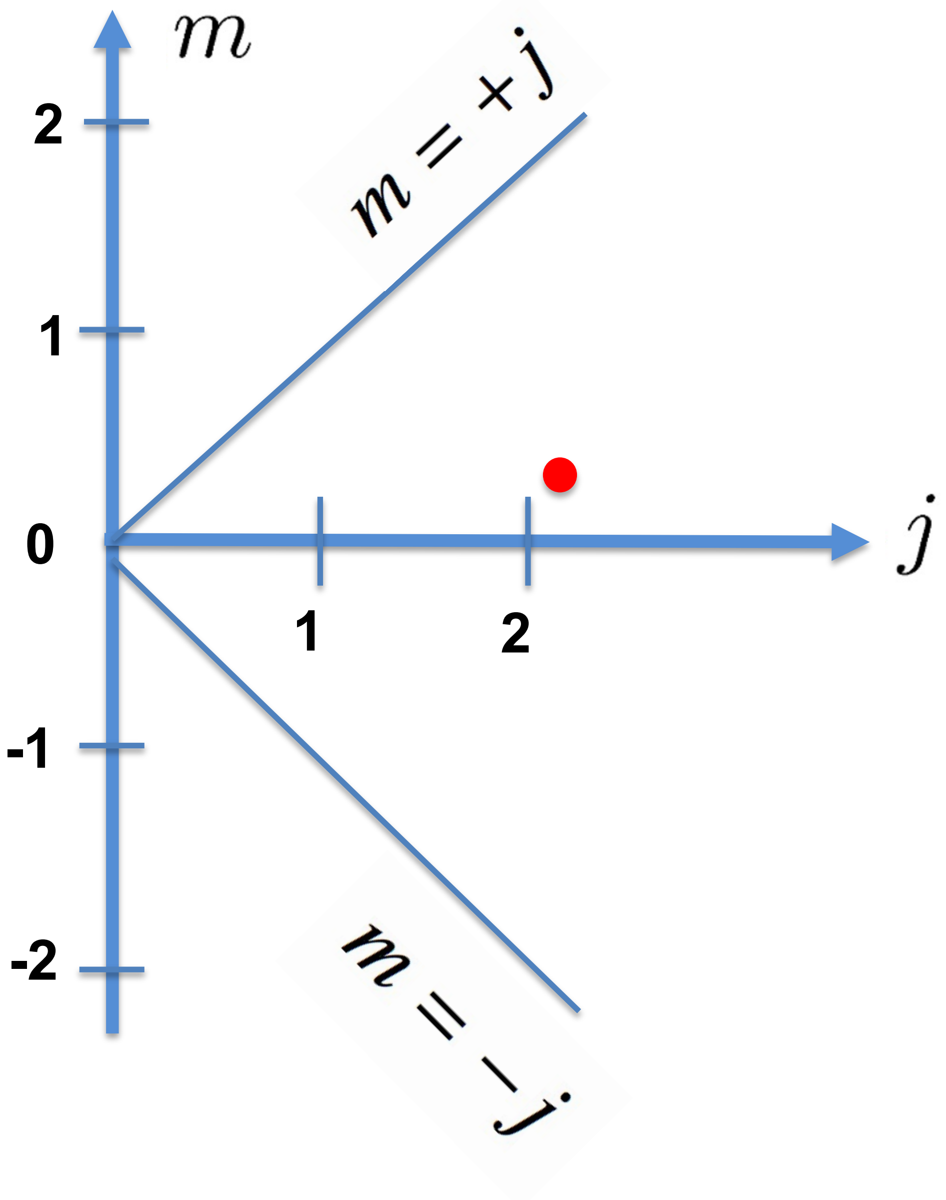
In summary

$$|\psi\rangle \in \mathcal{E}_{j,m} \qquad \hat{J}_{\pm}|\psi\rangle \in \mathcal{E}_{j,m\pm 1} \qquad -j \leq m \leq j$$

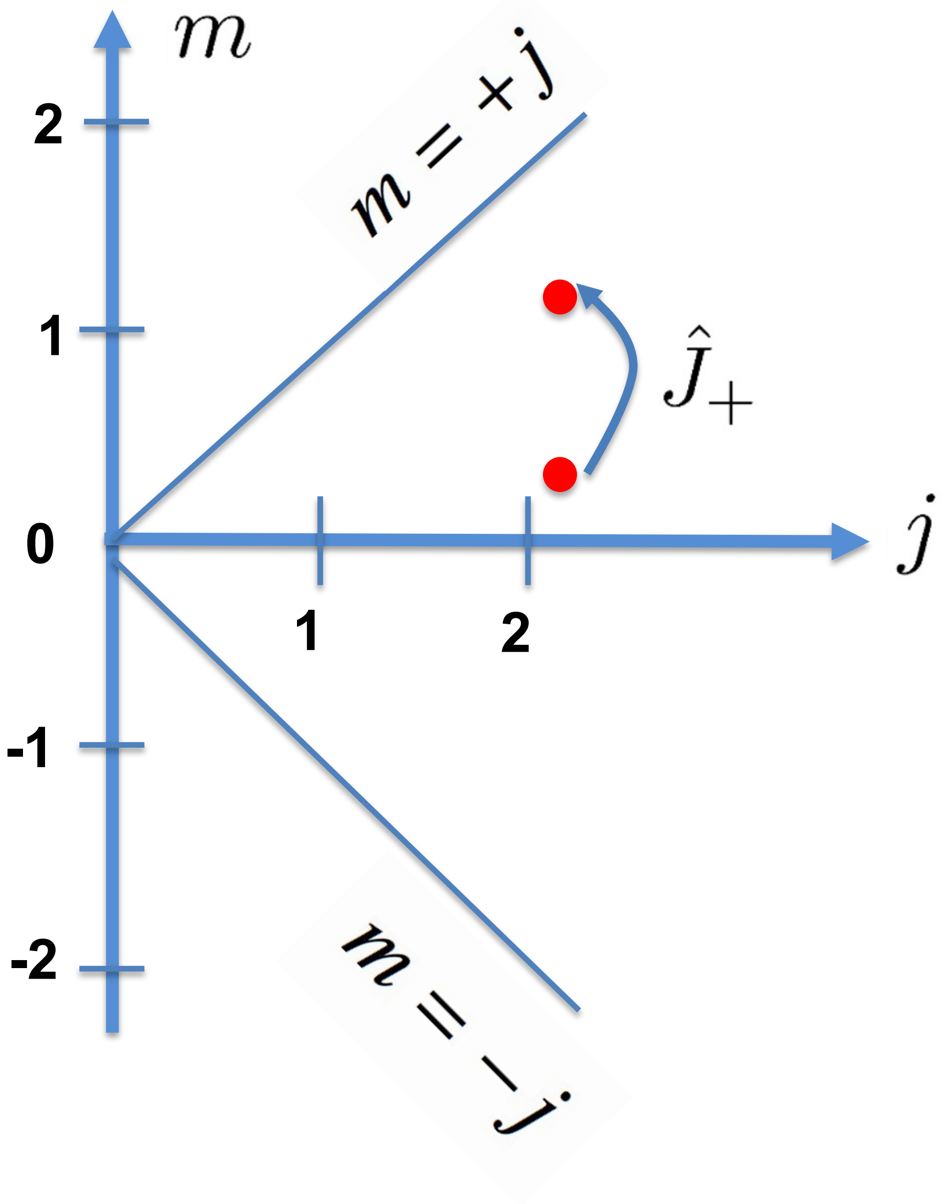
$$||\hat{J}_{\pm}|\psi\rangle||^2 = (j(j+1) - m(m \pm 1))\,\hbar^2$$

$||\hat{J}_{+}|\psi\rangle|| = 0$ **iff** $m = j$ $\qquad$ $||\hat{J}_{-}|\psi\rangle|| = 0$ **iff** $m = -j$

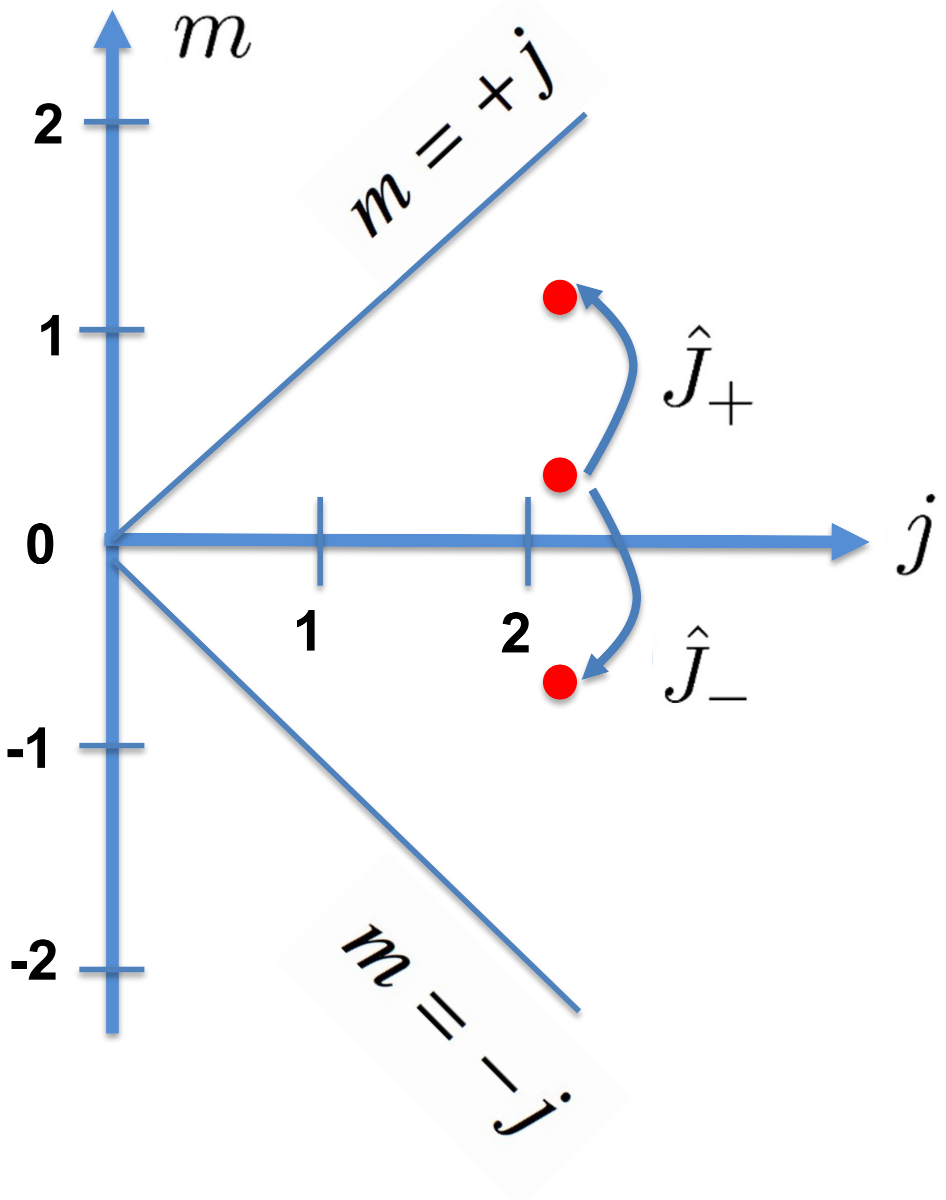
What values for m and j?



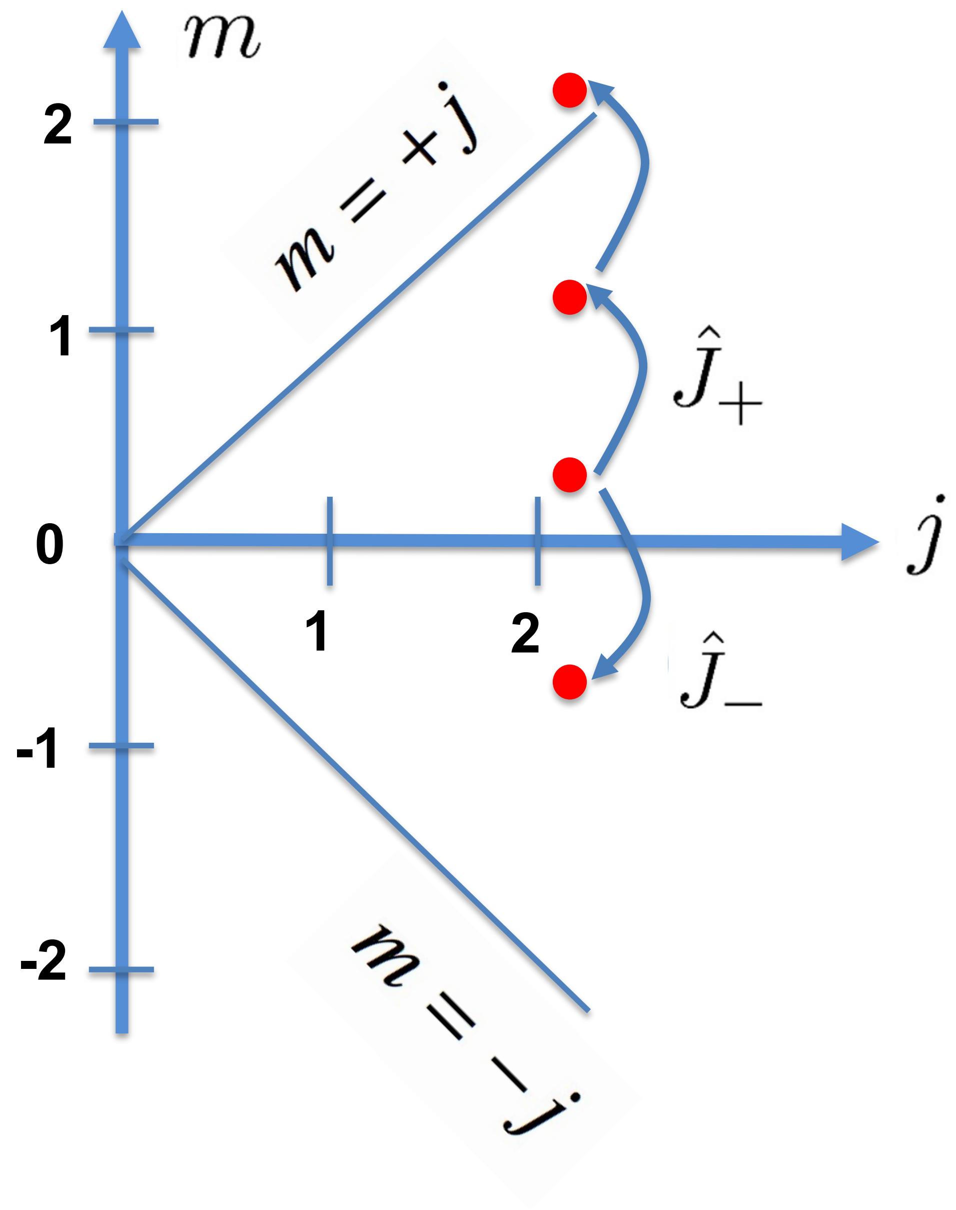
What values for m and j?



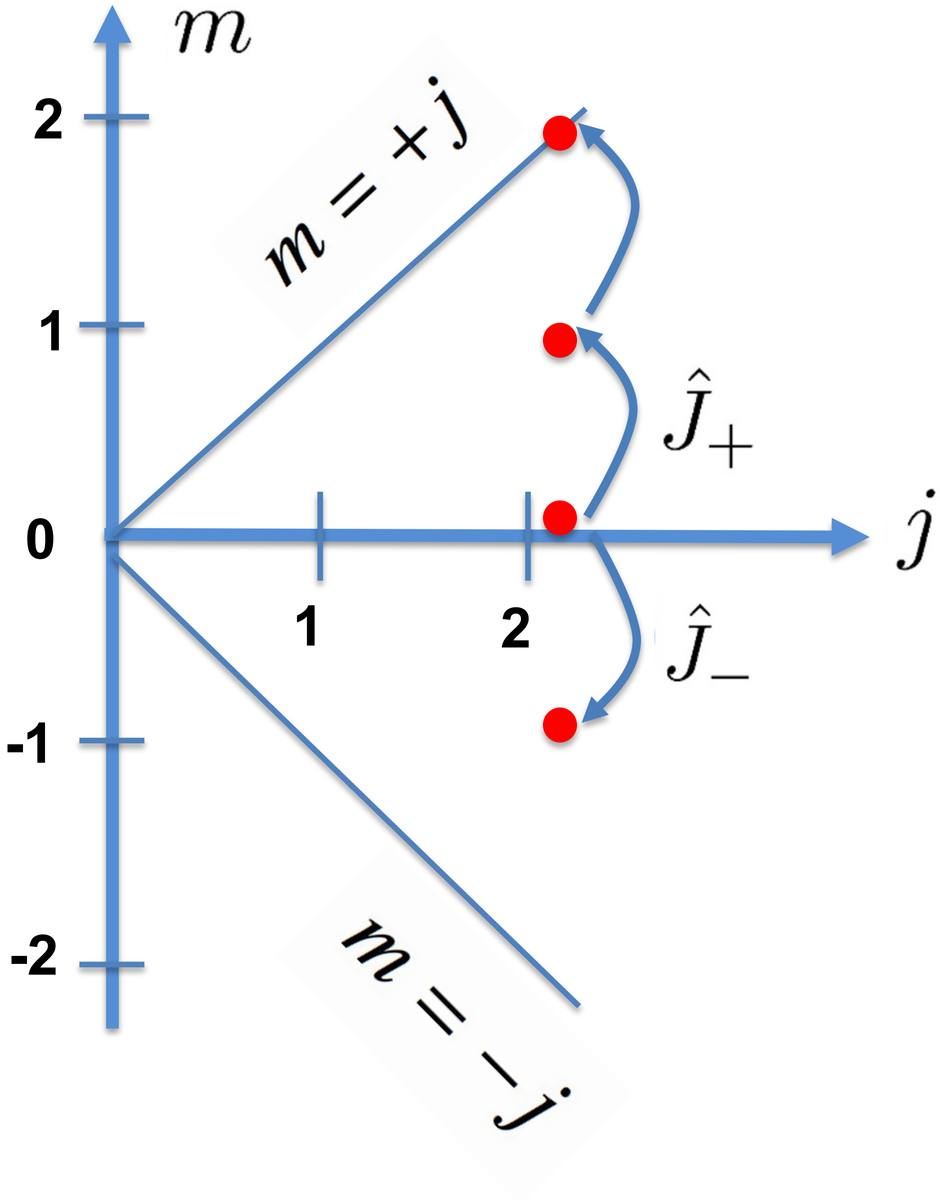
What values for m and j?



What values for m and j?

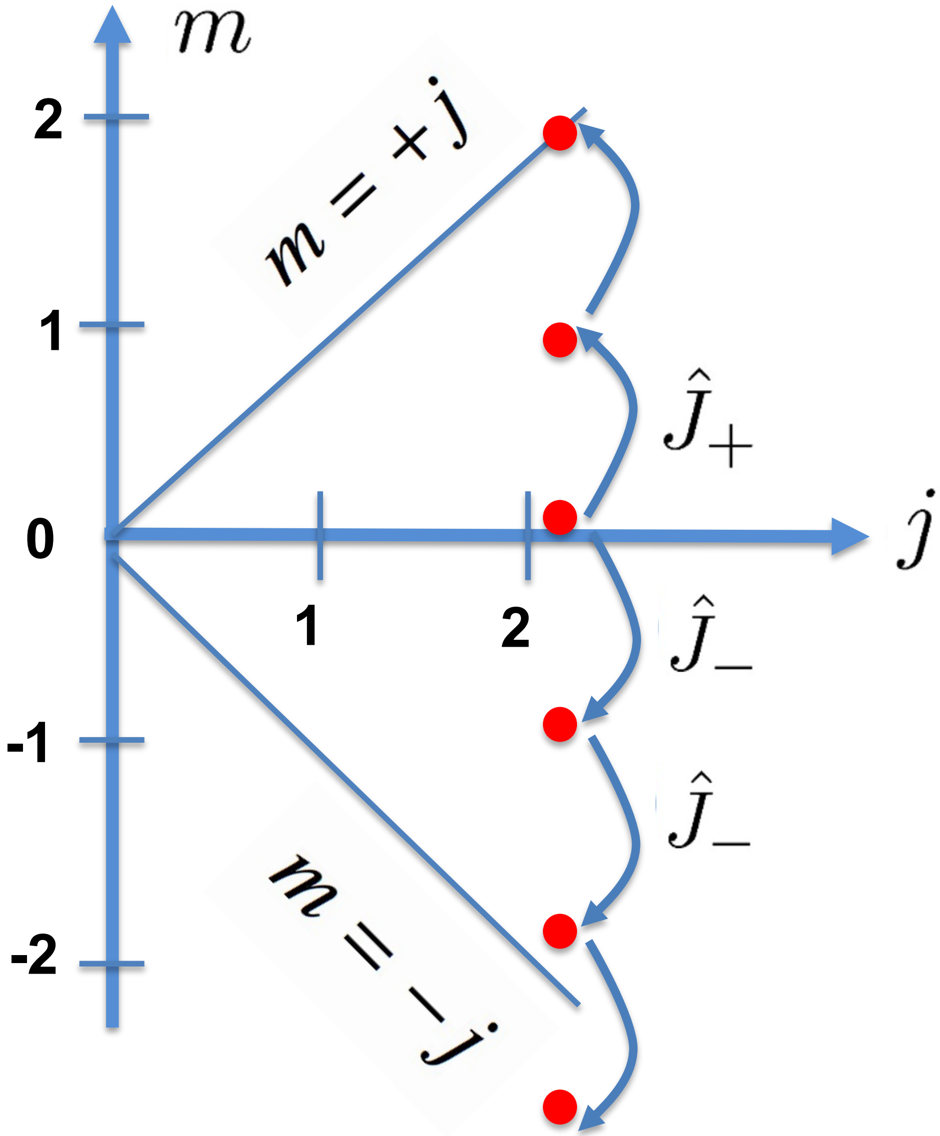


What values for m and j?



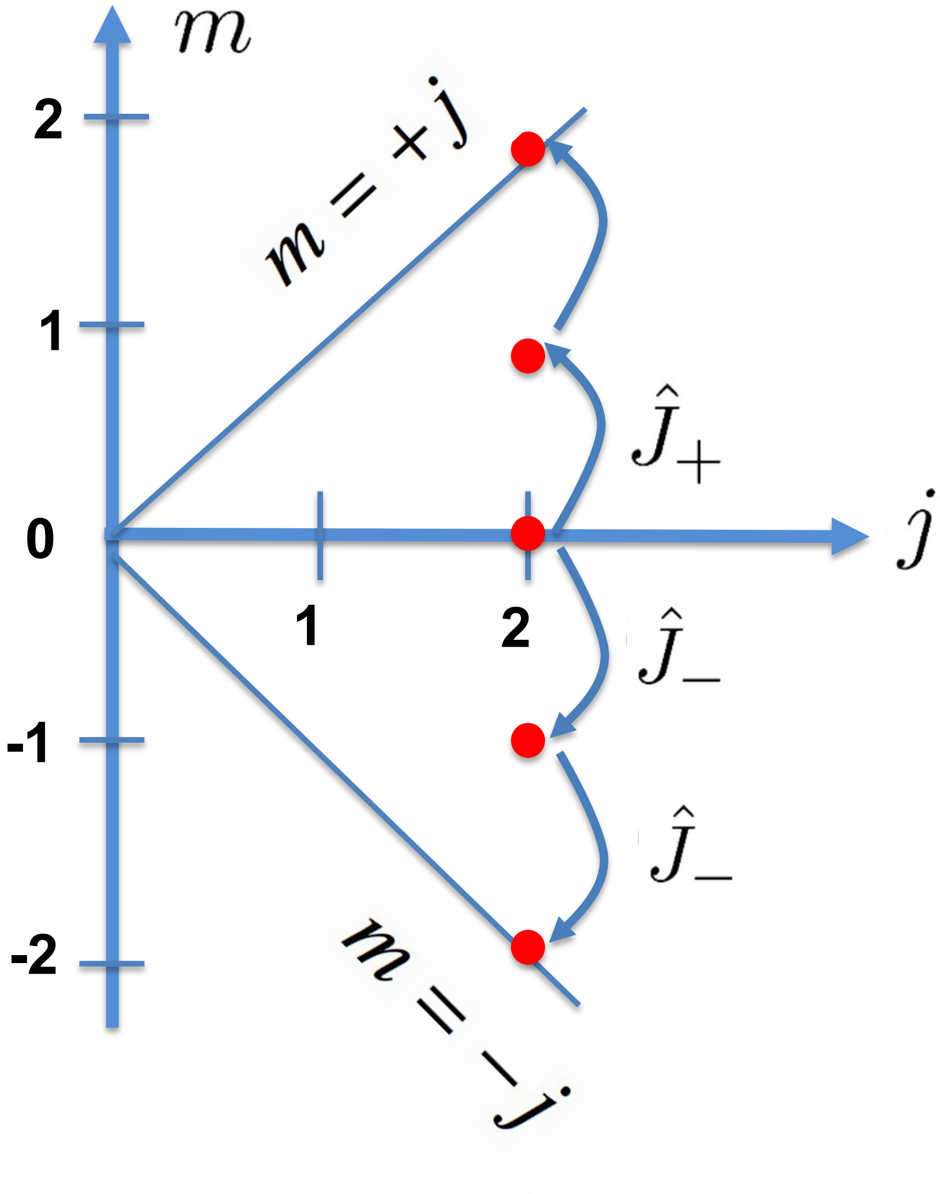
$$\exists N \in \mathbb{N} \quad m + N = j$$

What values for m and j?



$$\exists N \in \mathbb{N} \quad m + N = j$$

What values for m and j?



$$\exists N \in \mathbb{N} \qquad m + N = j$$

$$\exists N' \in \mathbb{N} \qquad m - N' = -j$$

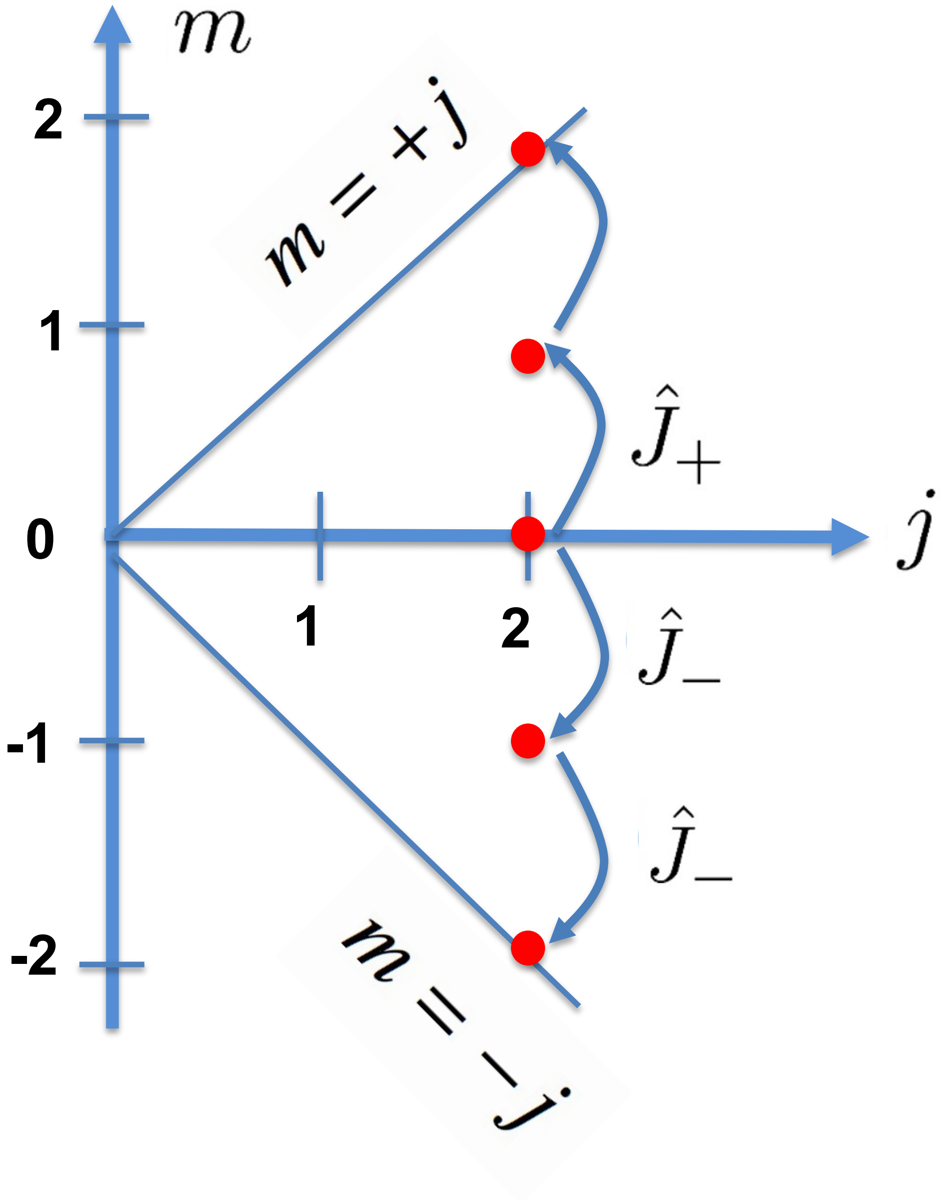
$$2j = N + N'$$

$$2j \in \mathbb{N} \qquad j - m \in \mathbb{N}$$

$$j \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\right\}$$

$$m \in \{-j, -j+1, \ldots, j\}$$

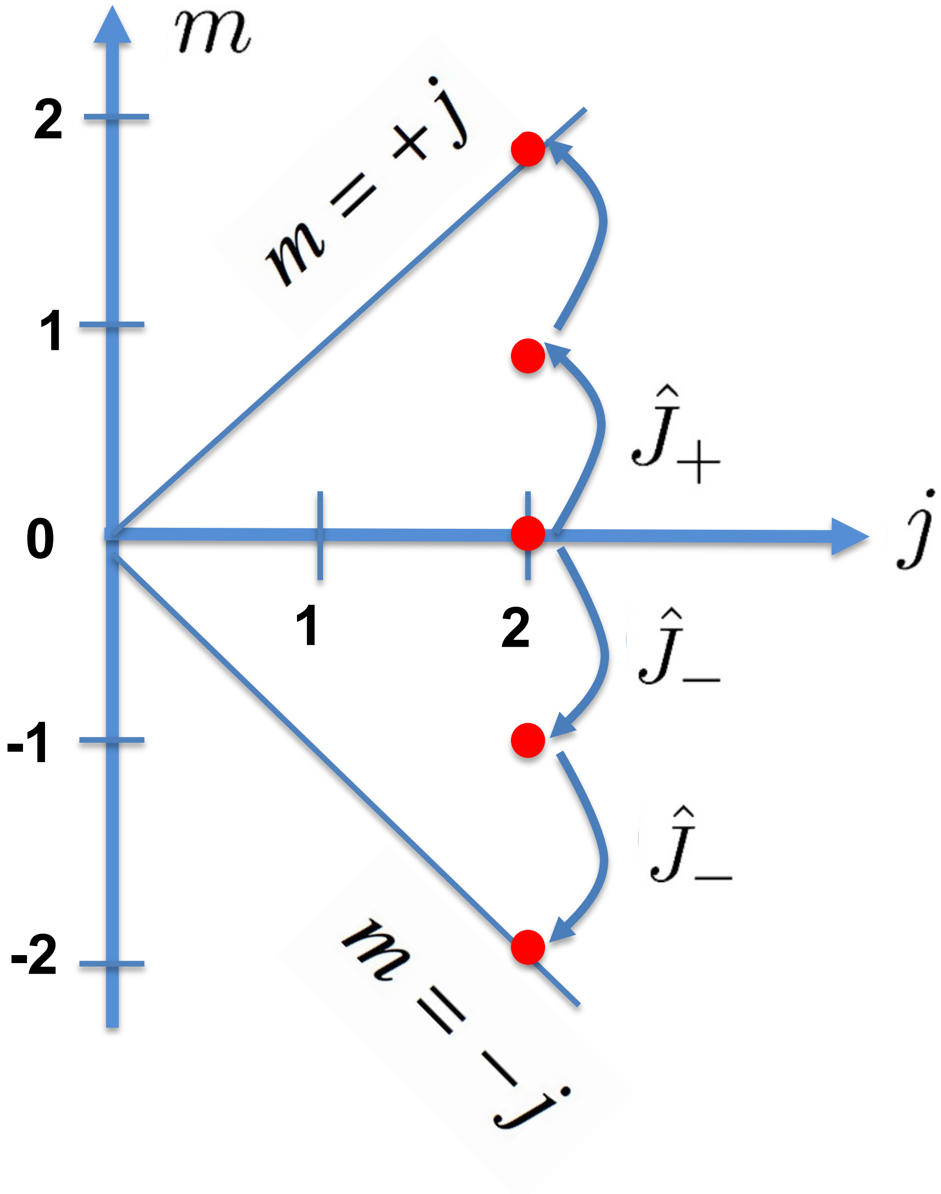
What values for m and j?



$$\exists N \in \mathbb{N} \quad m + N = j$$

$$\exists N' \in \mathbb{N} \quad m - N' = -j$$

What values for m and j?



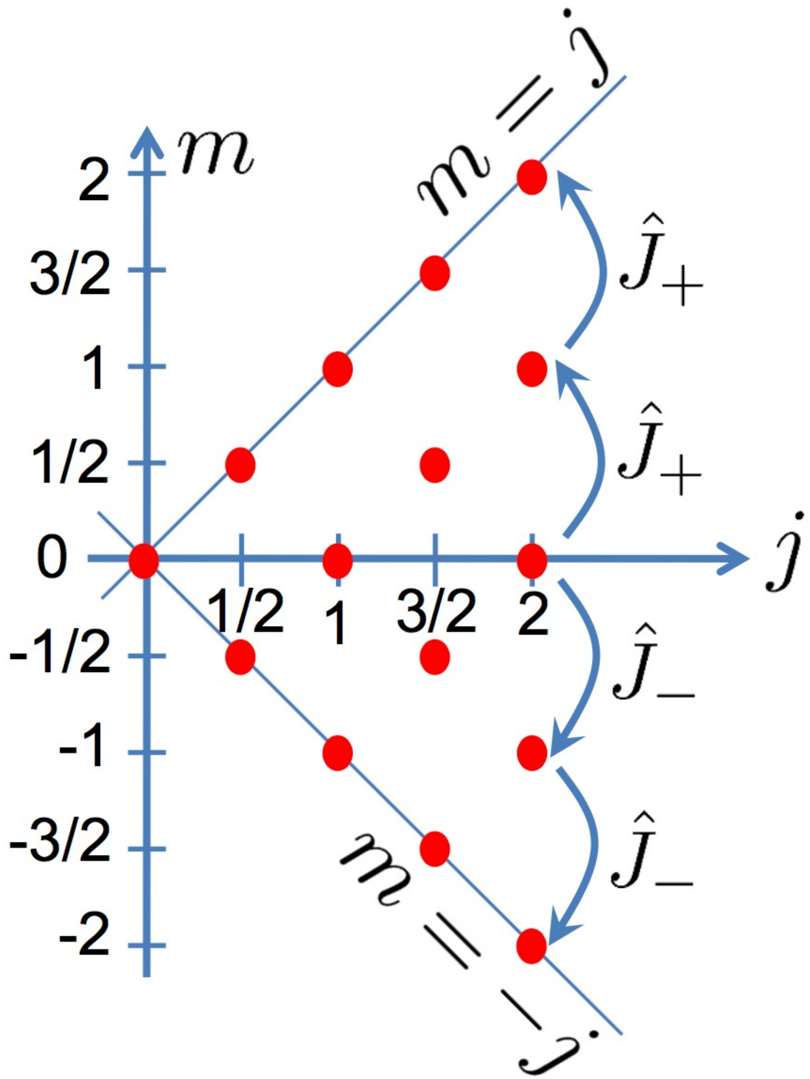
$$\exists N \in \mathbb{N} \quad m + N = j$$

$$\exists N' \in \mathbb{N} \quad m - N' = -j$$

$$2j = N + N'$$

$$2j \in \mathbb{N} \qquad j - m \in \mathbb{N}$$

What values for m and j?



$$\exists N \in \mathbb{N} \quad m + N = j$$

$$\exists N' \in \mathbb{N} \quad m - N' = -j$$

$$2j = N + N'$$

$$2j \in \mathbb{N} \qquad j - m \in \mathbb{N}$$

$$j \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\right\}$$

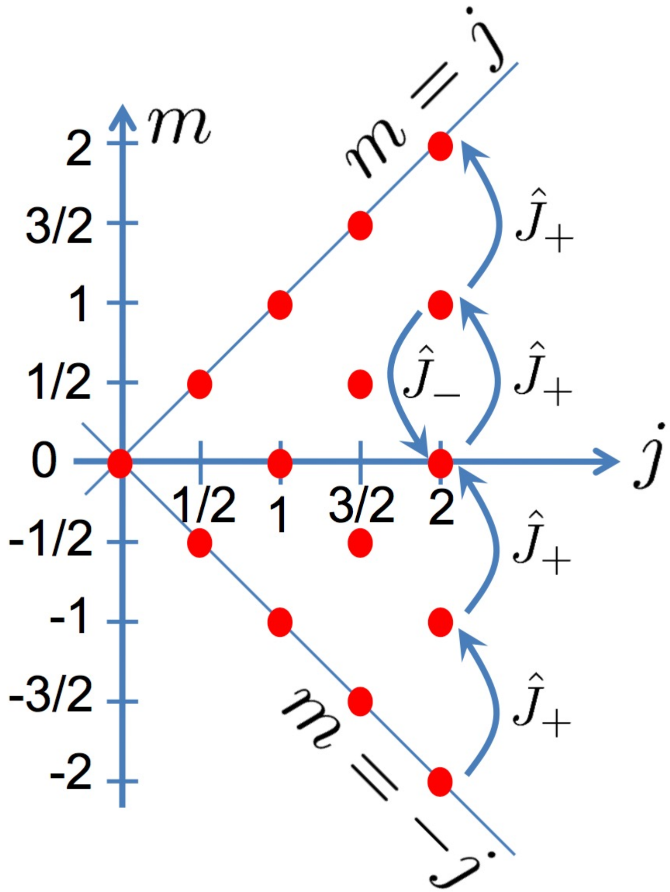
$$m \in \{-j, -j+1, \ldots, j\}$$

Eigenstates of $\left\{\hat{J}^2, \hat{J}_z\right\}$

Consider the standard basis $\left\{|n, j, m\rangle\right\}$

$$dim\ \mathcal{E}_{j,m} \geq 1$$

$$|n, j, m+1\rangle = \frac{\hat{J}_+|n, j, m\rangle}{\hbar\sqrt{j(j+1) - m(m+1)}}$$



$$\hat{J}^2|n, j, m\rangle = j(j+1)\hbar^2|n, j, m\rangle$$

$$\hat{J}_z|n, j, m\rangle = m\hbar|n, j, m\rangle$$

$$j \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...\right\}$$

$$m \in \{-j, -j+1, ..., j\}$$

$$\hat{J}_\pm|n, j, m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\hbar|n, j, m\pm 1\rangle$$

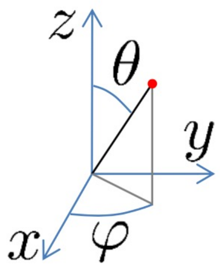
3.
Application to the orbital angular momentum

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

$$\hat{\vec{L}} \times \hat{\vec{L}} = i\hbar\hat{\vec{L}}$$

Operators in spherical coordinates

Using spherical coordinates we can write



$$\left[\hat{R}_{z,\alpha}\psi\right](r,\theta,\varphi) = \psi(r,\theta,\varphi-\alpha) \approx \psi(r,\theta,\varphi) - \alpha\frac{\partial\psi}{\partial\varphi}$$

$$\hat{R}_{z,\alpha} \approx \left(\hat{I} - \frac{i\alpha}{\hbar}\hat{L}_z\right)$$

$$\boxed{\hat{L}_z\psi(r,\theta,\varphi) = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}\psi(r,\theta,\varphi)}$$

Expressions for other coordinates

$$\hat{L}_x\psi(r,\theta,\varphi) = i\hbar\left(\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\psi(r,\theta,\varphi)$$

$$\hat{L}_y\psi(r,\theta,\varphi) = i\hbar\left(-\cos\varphi\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right)\psi(r,\theta,\varphi)$$

$$\hat{L}_\pm\psi(r,\theta,\varphi) = \hbar e^{\pm i\varphi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right)\psi(r,\theta,\varphi)$$

$$\hat{L}^2\psi(r,\theta,\varphi) = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\psi(r,\theta,\varphi)$$

Radial and angular functions

$$\hat{L}^2\psi(r,\theta,\varphi) = \ell(\ell+1)\hbar^2\psi(r,\theta,\varphi) \qquad \hat{L}_z\psi(r,\theta,\varphi) = m\hbar\psi(r,\theta,\varphi)$$

$$-\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\psi(r,\theta,\varphi) = \ell(\ell+1)\psi(r,\theta,\varphi)$$

$$-i\frac{\partial}{\partial\varphi}\psi(r,\theta,\varphi) = m\psi(r,\theta,\varphi)$$

Note that the radial variable r is not involved in the differential equations

An eigenvector of {L^2,L_z } is such as $\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$

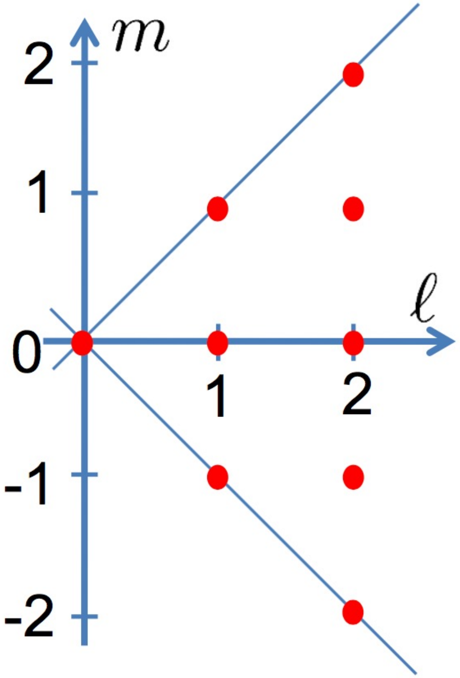
$$\langle\psi|\psi\rangle = \underbrace{\int_0^\infty |R(r)|^2 r^2 dr}_{=1} \underbrace{\int_0^\pi \int_0^{2\pi} |Y(\theta,\varphi)|^2 \sin\theta d\theta d\varphi}_{=1}$$

Eigenvalues of $\left\{\hat{L}^2, \hat{L}_z\right\}$

$$\hat{L}_z Y(\theta,\varphi) = m\hbar Y(\theta,\varphi) \qquad \Rightarrow \frac{\partial Y(\theta,\varphi)}{\partial \varphi} = imY(\theta,\varphi)$$

$$Y(\theta,\varphi) = F(\theta)\exp(im\varphi)$$

But : $Y(\theta,\varphi+2\pi) = Y(\theta,\varphi) \quad \Rightarrow \quad m$ entier $\quad \Rightarrow \quad \ell$ **integer**



$$\ell \in \mathbb{N}$$

$$m \in \{-\ell, -\ell+1, ..., \ell\}$$

Spherical harmonics $Y_{l,m}(\theta,\varphi)$

$$\boxed{Y_{\ell,m}(\theta,\varphi) = F_{\ell,m}(\theta)\exp(im\varphi)}$$

$m = -\ell \qquad \hat{L}_- Y_{\ell,-\ell}(\theta,\varphi) = \hat{L}_- F_{\ell,-\ell}(\theta) e^{-i\ell\varphi} = 0$

$\hat{L}_-$ is a first order linear differential operator → unique solution

We can prove $F_{\ell,-\ell}(\theta) \propto \sin^{\ell}\theta$ $\qquad \boxed{Y_{\ell,-\ell}(\theta,\varphi) \propto \sin^{\ell}\theta e^{-i\ell\varphi}}$

Using a recursive relationship and using L_+, we get

$$\boxed{Y_{\ell,m+1}(\theta,\varphi) = \frac{\hat{L}_+ Y_{\ell,m}(\theta,\varphi)}{\hbar\sqrt{\ell(\ell+1) - m(m+1)}}}$$

Geometrical representation

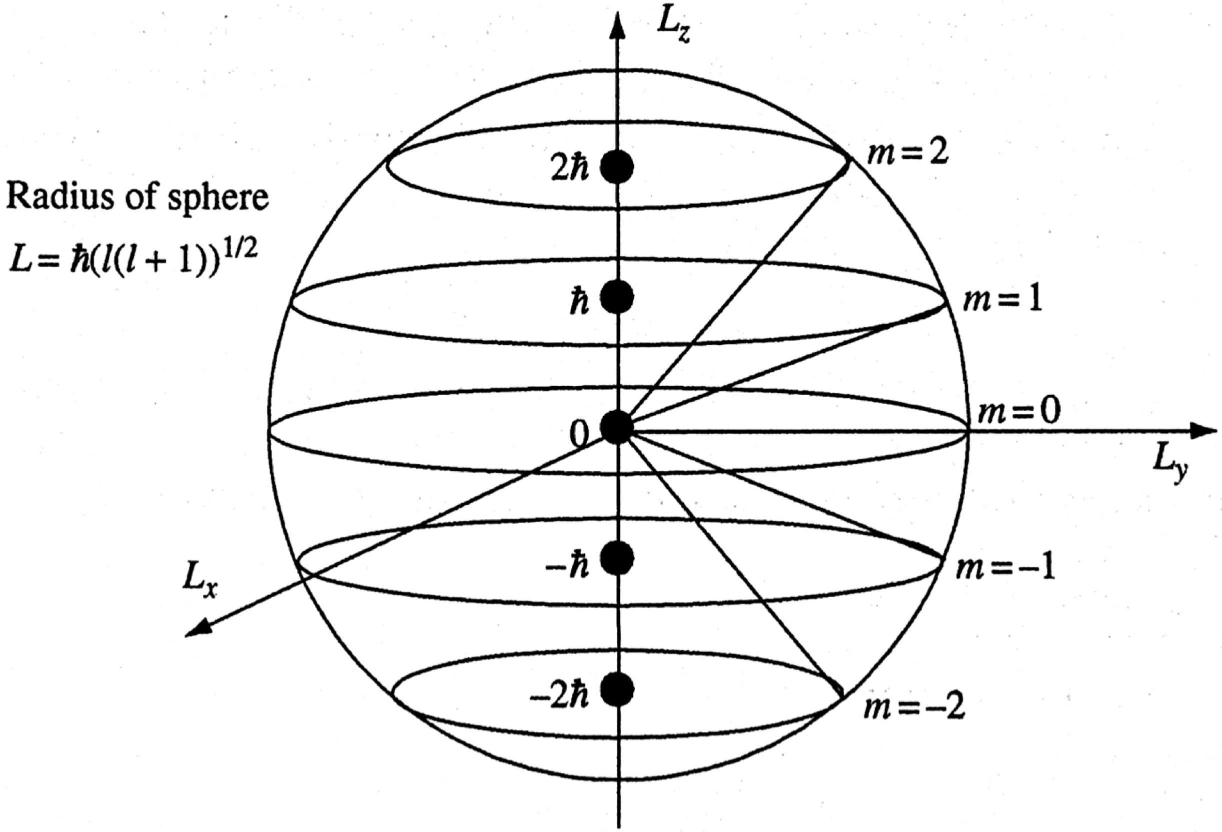


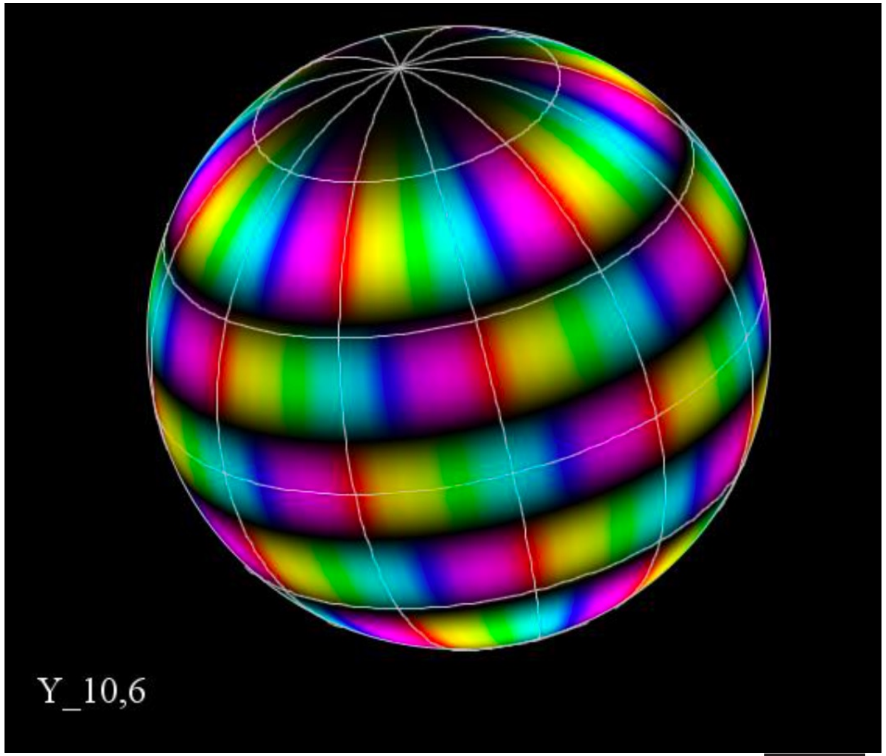
Fig. 11.3 Geometrical representation of quantized angular momentum for a state with $l = 2$. The z-component of angular momentum is quantized such that $L_z = m\hbar$ where integer m has values $-l \leq m \leq l$. One may think of the state existing with indeterminate values of L_x and L_y at the bisection of the (L_x, L_y) plane that passes through the quantized value $L_z = m\hbar$ with the sphere of quantized radius $L = \hbar(l(l+1))^{1/2}$.

Spherical harmonics $Y_{l,m}(\theta,\varphi)$

$F_{l,m}(\theta)$ is a real function with $l-|m|$ nodes in the interval $]0\,,\pi[$

$$\forall Y : (\theta,\varphi) \mapsto Y(\theta,\varphi) \in \mathbb{C}, \exists\{c_{\ell,m}\}$$

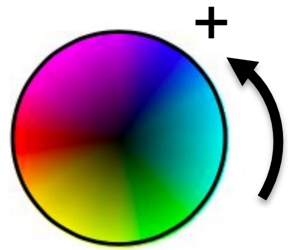
$$Y(\theta,\varphi) = \sum_{\ell,m} c_{\ell,m} Y_{\ell,m}(\theta,\varphi)$$



Along the parallels, we observe the dependence with the azimuth angle which allows to determine m

Along the meridians, the number of nodes allows to determine l when varying the polar angle

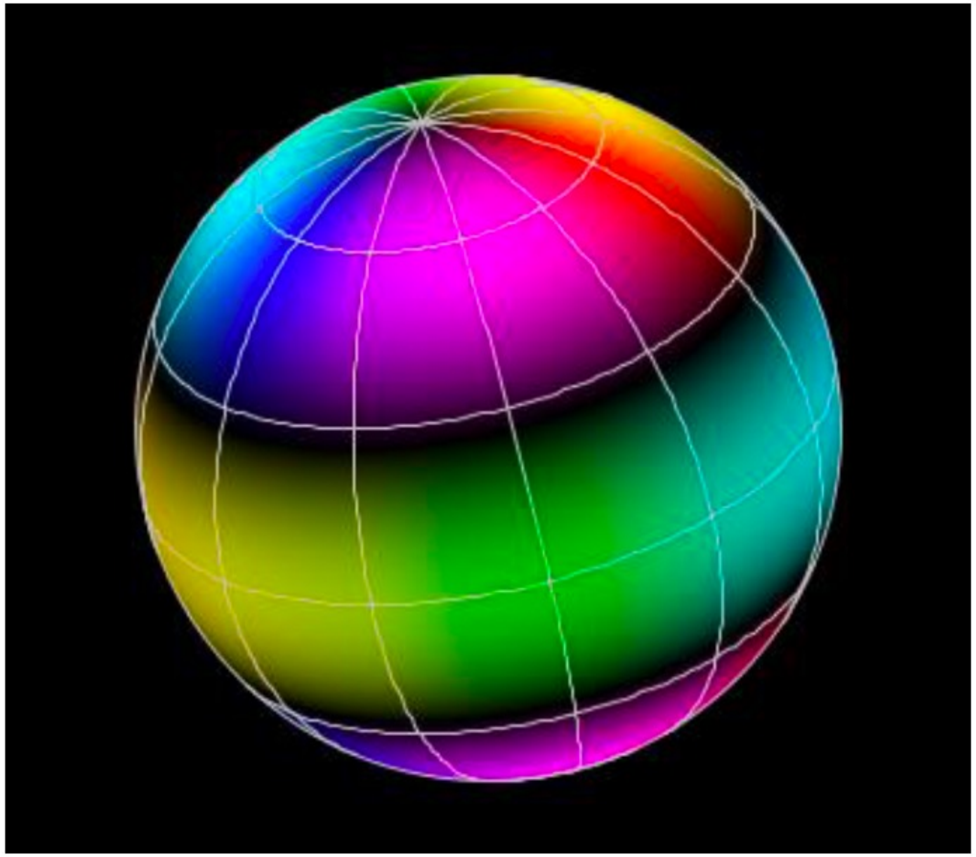
Quiz 8



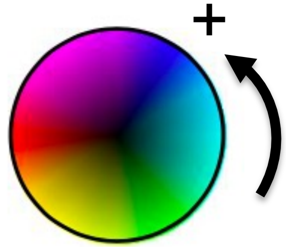
Find the spherical harmonic $Y_{l,m}(\theta, \varphi)$

A. $\ell = 0$
B. $\ell = 1$
C. $\ell = 2$
D. $\ell = 3$

E. $m = -2$
F. $m = -1$
G. $m = 0$
H. $m = 1$
I. $m = 2$



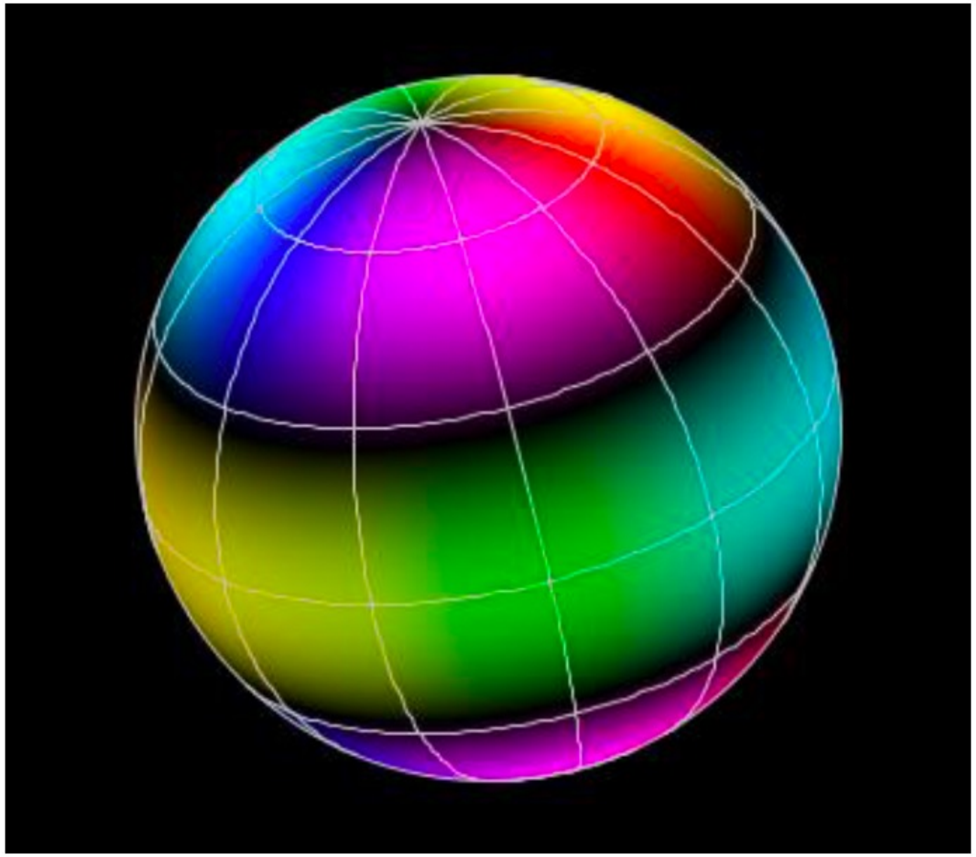
Quiz 8



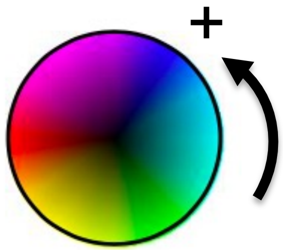
Find the spherical harmonic $Y_{l,m}(\theta, \varphi)$

A. $\ell = 0$
B. $\ell = 1$
C. $\ell = 2$
D. $\ell = 3$

E. $m = -2$
F. $m = -1$
G. $m = 0$
H. $m = 1$
I. $m = 2$



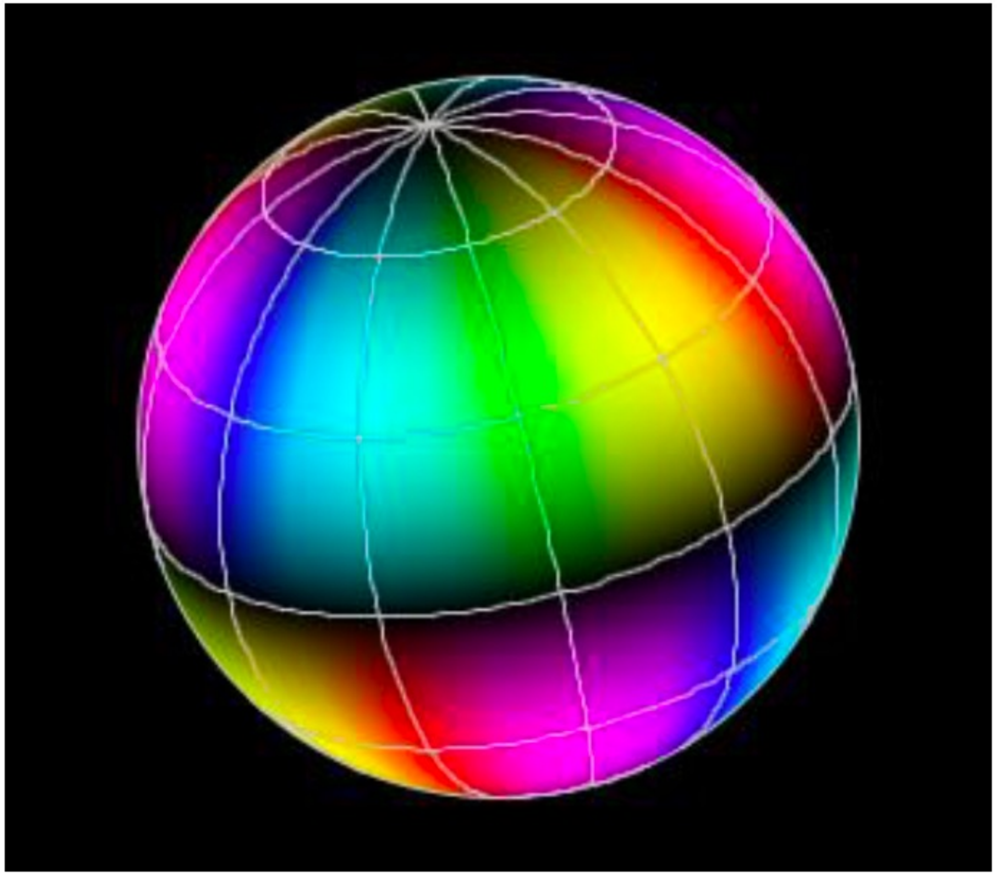
Quiz 9



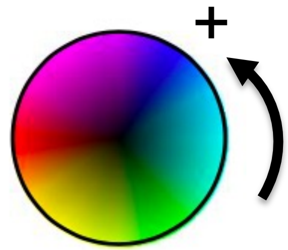
Find the spherical harmonic $Y_{l,m}(\theta, \varphi)$

A. $\ell = 0$
B. $\ell = 1$
C. $\ell = 2$
D. $\ell = 3$

E. $m = -2$
F. $m = -1$
G. $m = 0$
H. $m = 1$
I. $m = 2$



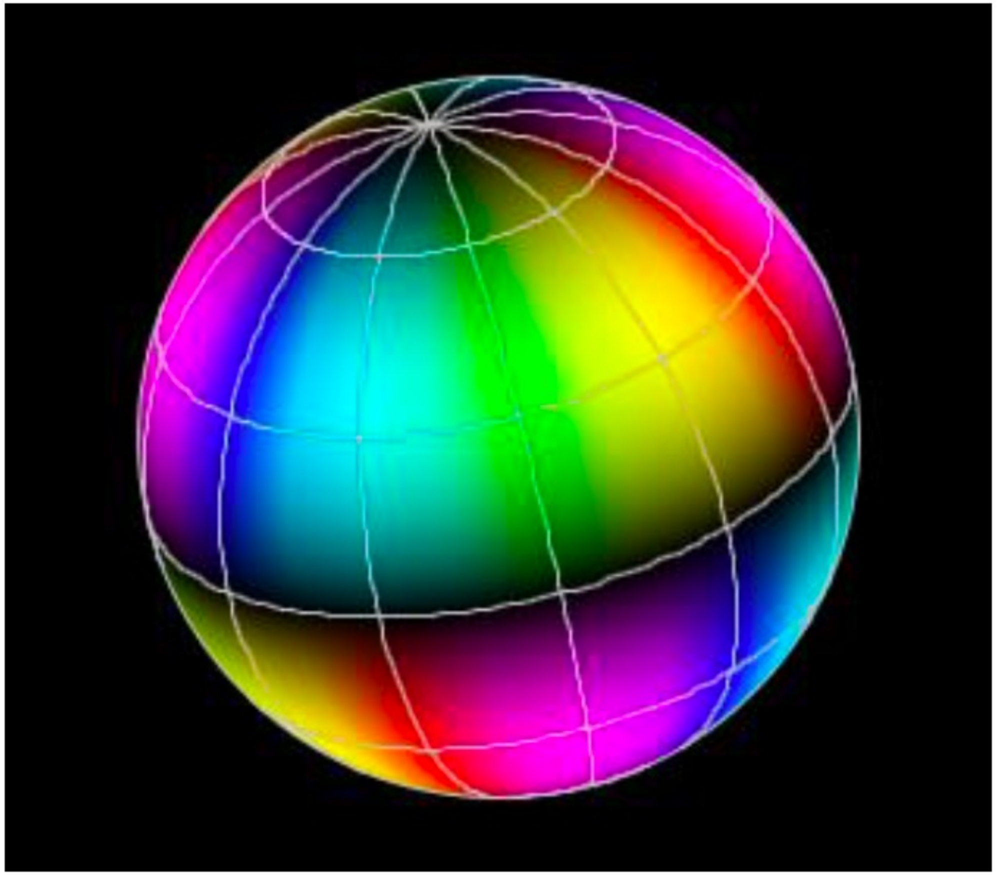
Quiz 9



Find the spherical harmonic $Y_{l,m}(\theta,\varphi)$

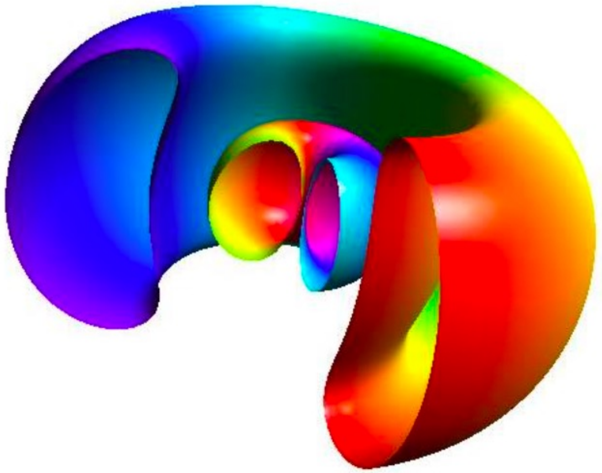
A. $\ell = 0$
B. $\ell = 1$
C. $\ell = 2$
D. $\ell = 3$

E. $m = -2$
F. $m = -1$
G. $m = 0$
H. $m = 1$
I. $m = 2$



Section 9

The hydrogen atom



Introduction

Spectrum with discrete lines (Rydberg, Balmer)

$$\frac{1}{\lambda} = Ry\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

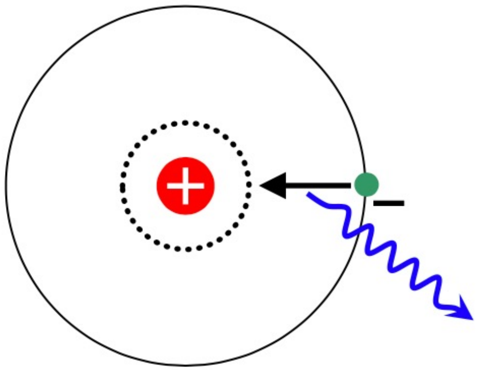
n_1, n_2 : positive integers

Ry : Rydberg

Planetary models (Perrin, Rutherford)

The classical physics predicts that the electron will fall onto the nucleus because a moving and accelerated charge radiates

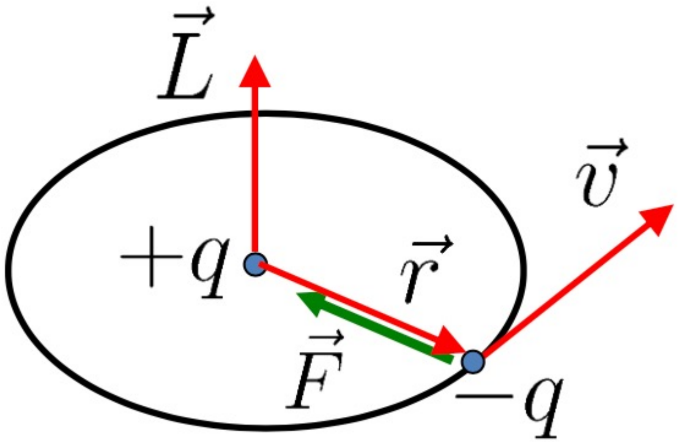
→ Bohr: only certain orbits are allowed



Bohr's model

Consider a circular trajectory

$$\frac{m_e v^2}{r} = \frac{e^2}{r^2} \Rightarrow m_e v^2 = \frac{e^2}{r}$$



w/ $e^2 = \dfrac{q^2}{4\pi\epsilon_0}$

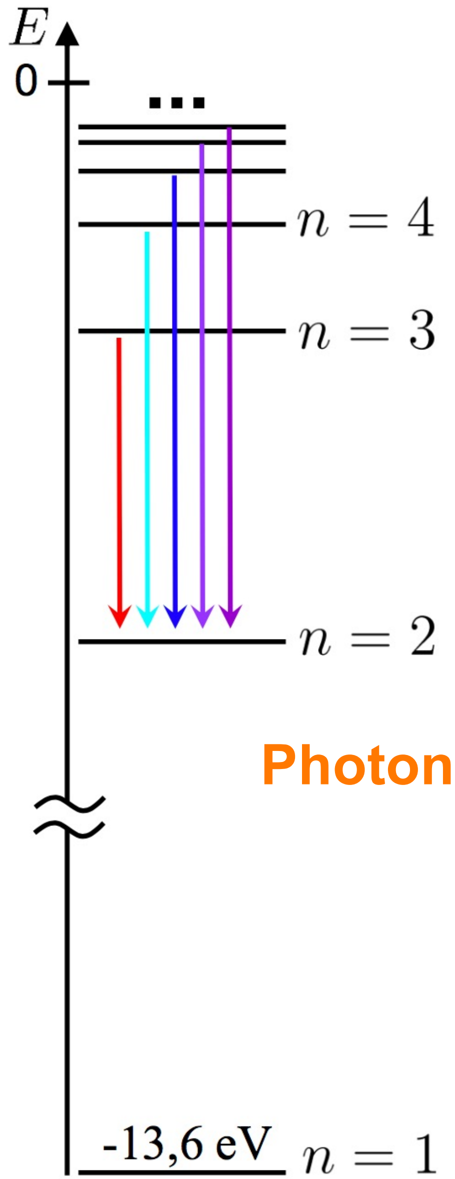
Quantization of angular momentum

$$L_z = r m_e v = n\hbar \qquad n = 1, 2, \ldots$$

$$v_n = \frac{1}{n}\frac{e^2}{\hbar} = \alpha \frac{c}{n}$$ w/ α the fine-structure constant $\alpha = \dfrac{e^2}{\hbar c} \approx \dfrac{1}{137}$

$$r_n = \frac{n\hbar}{m_e v_n} = n^2 a_1$$ w/ a_1 the Bohr radius $a_1 = \dfrac{\hbar^2}{m_e e^2} \approx 0.053\ nm$

Bohr's model



Total energy $E_n = \frac{1}{2}m_e v_n^2 - \frac{e^2}{r_n} = \boxed{-\frac{E_I}{n^2}}$

$$E_I = \frac{m_e e^4}{2\hbar^2} = \frac{\hbar^2}{2m_e a_1^2} \approx 13{,}6 \text{ eV}$$

Photon energy associated to the transition $n_1 \longrightarrow n_2$

$$h\nu = E_I\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$$

The model perfectly predicts the different energy levels but remains incomplete at the microscopic level (quantization not justified)

The Hydrogen atom in quantum mechanics

Two particles under the Coulomb interaction: proton + electron

As in classical mechanics, we can introduce the reduced mass to reduce the number of degrees of freedom (6 → 3)

$$\frac{1}{\mu} = \frac{1}{m_p} + \frac{1}{m_e} \approx \frac{1}{m_e}$$

Schrodinger equation

$$\hat{H} = \frac{\hat{p}^2}{2\mu} + V(\hat{r}) \quad \textbf{with} \quad V(r) = -\frac{e^2}{r}$$

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

The Coulomb potential is an example of what is known as a central potential or radial potential, one that depends only on the distance r to the origin

Motion in a central potential

Consider the Laplacian expressed in spherical coordinates

$$\left(-\frac{\hbar^2}{2\mu}\Delta + V(r)\right)\psi(r,\theta,\varphi) = E\,\psi(r,\theta,\varphi)$$

with

$$\Delta\psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2}\underbrace{\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right)}_{-\frac{\hat{L}^2}{\hbar^2}\psi}$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{2\mu r^2} + V(r)\right)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

Rotational Kinetic Energy

Motion in a central potential

$$\underbrace{\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hat{L}^2}{2\mu r^2} + V(r)\right)}_{\hat{H}}\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi)$$

Rotational invariance $[\hat{H}, \hat{L}_\alpha] = 0$

Complete set of commuting observables → common basis $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$

$$\psi(r,\theta,\varphi) = R(r)\, Y_{\ell,m}(\theta,\varphi)$$

$Y_{\ell,m}(\theta,\varphi)$ **: Spherical harmonics**

$$\hat{L}^2 Y_{\ell,m}(\theta,\varphi) = \ell(\ell+1)\hbar^2 Y_{\ell,m}(\theta,\varphi)$$

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r)\right)R(r)\cancel{Y_{\ell,m}(\theta,\varphi)} = ER(r)\cancel{Y_{\ell,m}(\theta,\varphi)}$$

The radial equation

$$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} + V(r)\right)R(r) = ER(r)$$

Reduced radial wavefunction $u(r) = r\,R(r)$ **with** $\int_0^\infty |u(r)|^2\,dr = 1$

Radial equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + V_{eff}(r)u(r) = Eu(r)$$

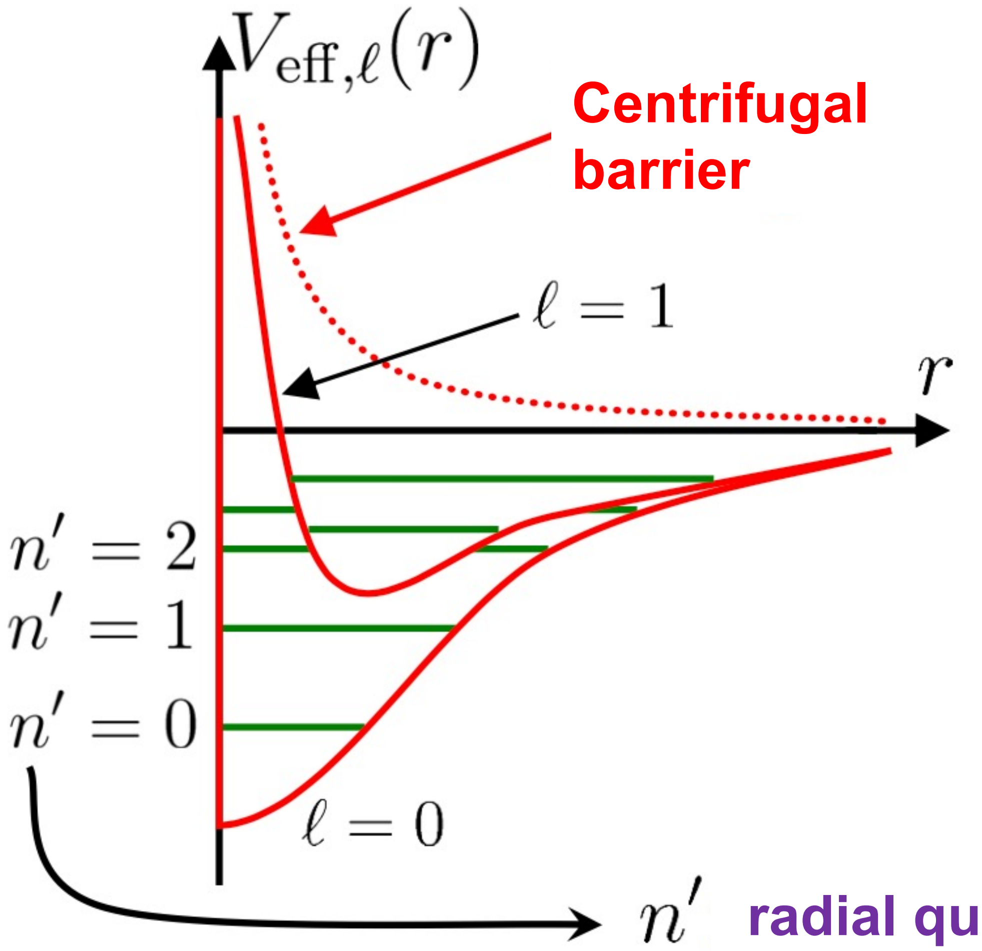
with $$V_{\mathrm{eff},\ell}(r) = V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}$$

3D→ 1D Schrodinger equation

But we get one equation for each value of l (e.g. multiple 1D problems)

This equation is independent of $m \in \{-\ell, -\ell+1, ..., \ell\}$

The radial equation



radial quantum number

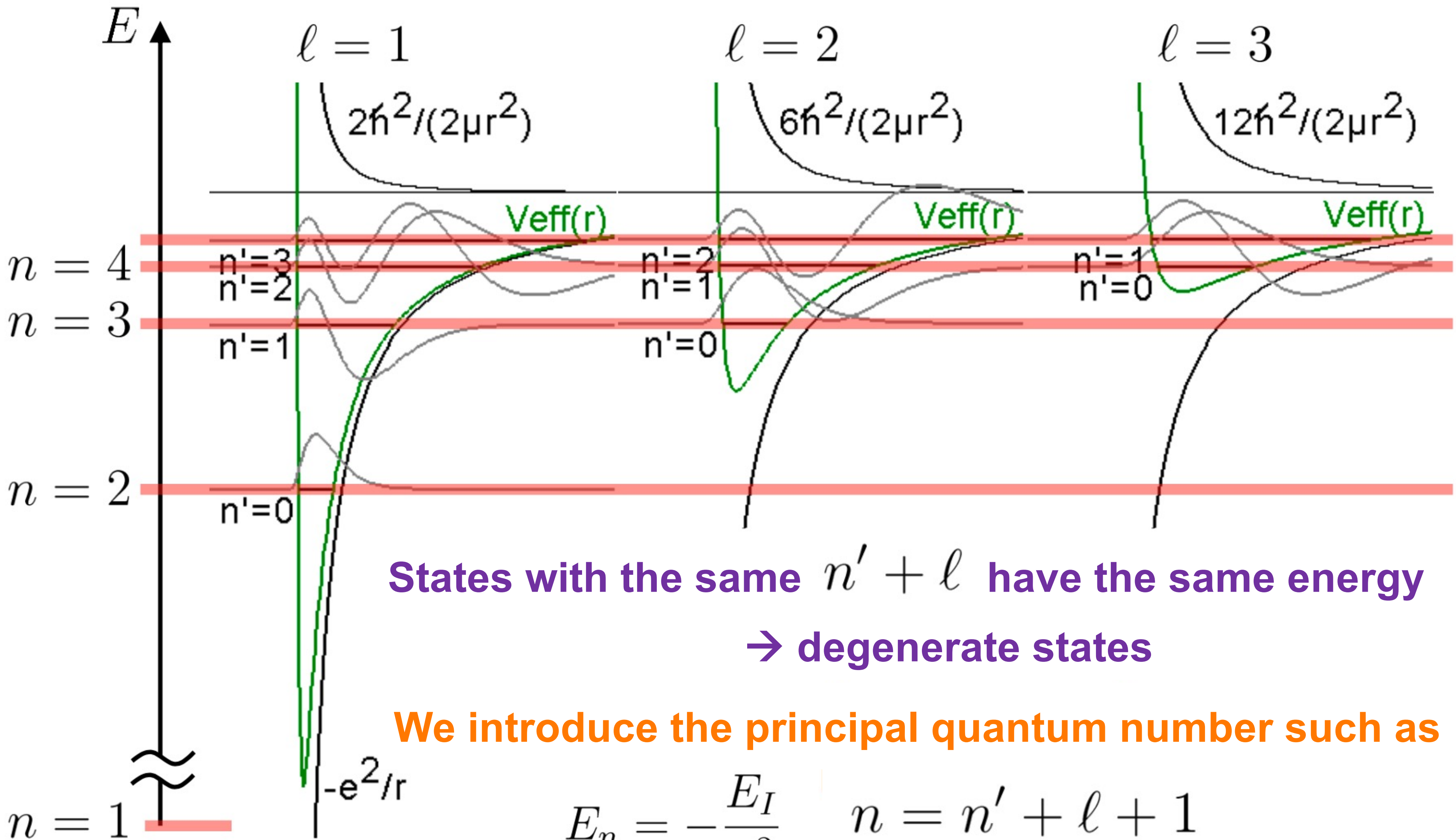
$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} + V_{eff}(r)u(r) = Eu(r)$$

$$V_{\mathrm{eff},\ell}(r) = V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}$$

2.
Determination of the eigenstates of the hydrogen atom

$$V_{\mathrm{eff},\ell}(r) = -\frac{e^2}{r} + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}$$

The principal quantum number



States with the same $n' + \ell$ have the same energy

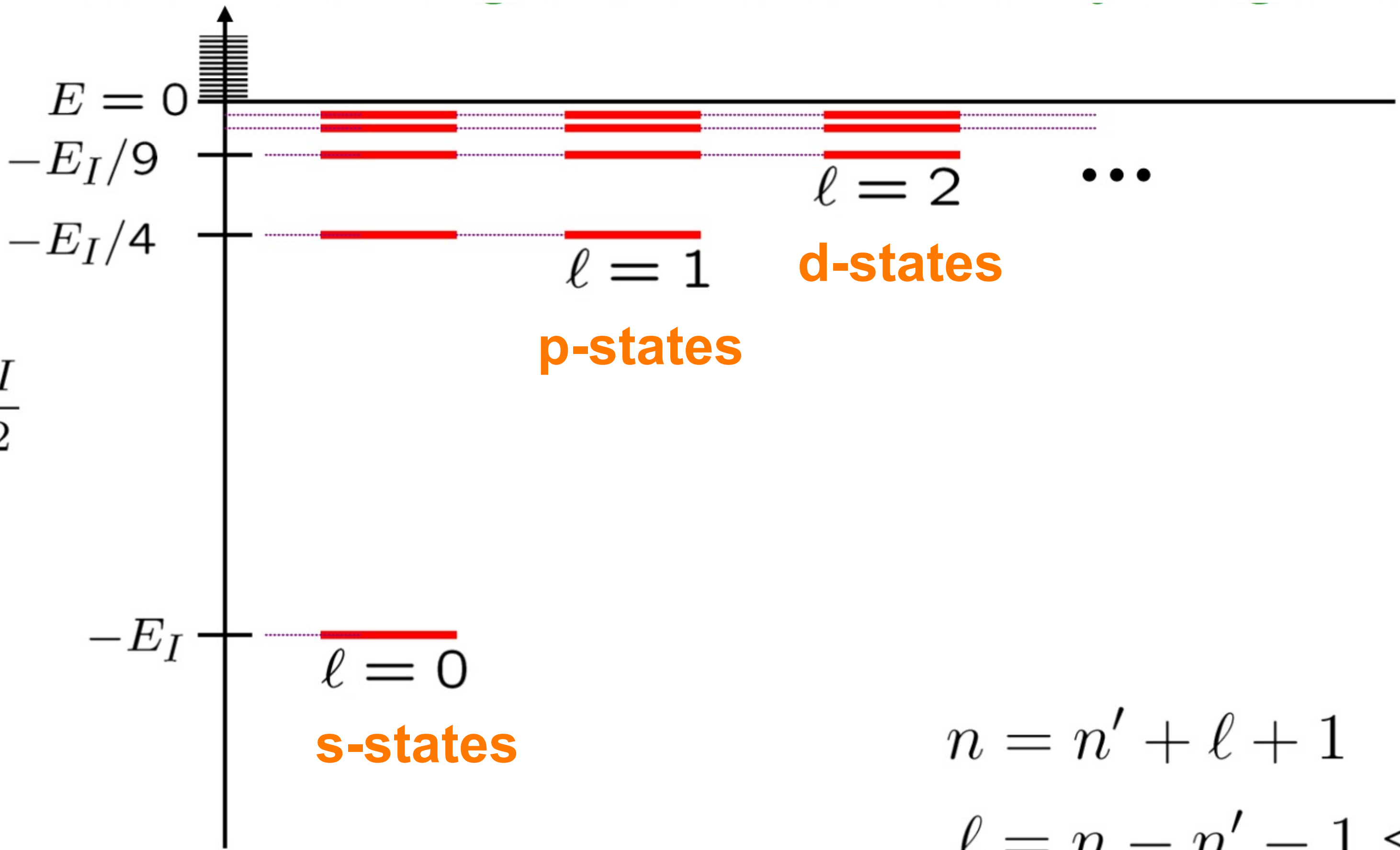
→ degenerate states

We introduce the principal quantum number such as

$$E_n = -\frac{E_I}{n^2} \qquad n = n' + \ell + 1$$

Energy levels of the Hydrogen atom

$$E_n = -\frac{E_I}{n^2}$$



$$n = n' + \ell + 1$$

$$\ell = n - n' - 1 \leq n - 1$$

For a given value of the energy E_n we have $\ell = 0, 1, ..., n-1$

The degeneracy of the level E_n i.e corresponding to the dimension of the vector subspace is $1 + 3 + ... + (2\ell + 1) + ... + (2n - 1) = n^2$

Degeneracy enhanced by 4 when considering electron and proton spins

Eigenstates

The eigenstates are represented by the ket-vector $|n, \ell, m\rangle$

$$\hat{H}|n, \ell, m\rangle = E_n|n, \ell, m\rangle \qquad E_n = -\frac{E_I}{n^2}$$

The wavefunction are $\psi_{n,\ell,m}(r, \theta, \varphi) = R_{n,\ell}(r) Y_{\ell,m}(\theta, \varphi)$

with $Y_{\ell,m}(\theta, \varphi) = F_{\ell,m}(\theta) \exp(im\varphi)$

$F_{l,m}(\theta)$ is a real function with $l - |m|$ nodes in $]0, \pi[$

For the radial function $R_{n\ell}(r)$ it is possible to show

$$R_{n\ell}(r) = \frac{u_{n\ell}(r)}{r} = [\text{polynomial function of degree } n'] \times r^{\ell} \exp\left(-\frac{r}{na_1}\right)$$

$R_{n\ell}(r)$ has n' nodes in $]0, +\infty[$ $\qquad n' = n - \ell - 1$

The radial functions

$$R_{10} = 2\left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-Zr/a_0}$$

$$R_{21} = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$$

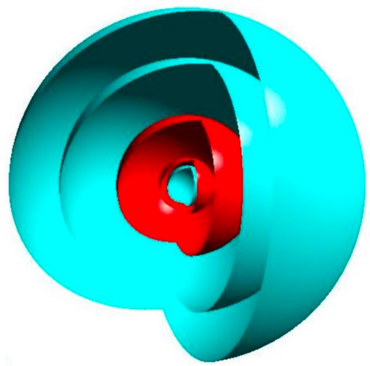
$$R_{20} = 2\left(\frac{Z}{2a_0}\right)^{\frac{3}{2}}\left(1-\frac{Zr}{2a_0}\right) e^{-Zr/2a_0}$$

$$R_{32} = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$$

$$R_{31} = \frac{4\sqrt{2}}{3}\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(\frac{Zr}{a_0}\right)\left(1-\frac{Zr}{6a_0}\right) e^{-Zr/3a_0}$$

$$R_{30} = 2\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}}\left(1-\frac{2Zr}{3a_0}+\frac{2\,(Zr)^2}{27a_0^2}\right) e^{-Zr/3a_0}$$

3.
Atomic orbitals



Representation of an atomic orbital

How can we represent the complex wavefunction $\psi(x,y,z)$?

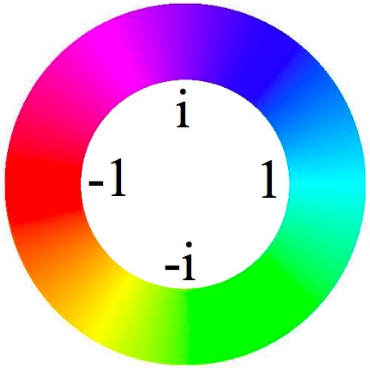
We represent isodensity surfaces defined $\left|\psi(x,y,z)\right| = \eta$

The constant η is a real number and choose such as

$$\iiint\limits_{|\psi(x,y,z)| \geq \eta} |\psi(x,y,z)|^2 dxdydz = \mathcal{P} \qquad \text{with for instance } \mathcal{P} = 0{,}5.$$

→ This gives the probability $\mathcal{P}$ to find the electron within the surface

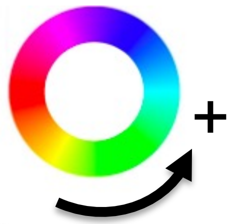
Then, we represent the phase and the complex wavefunction by using a color code



$\ell = 0$

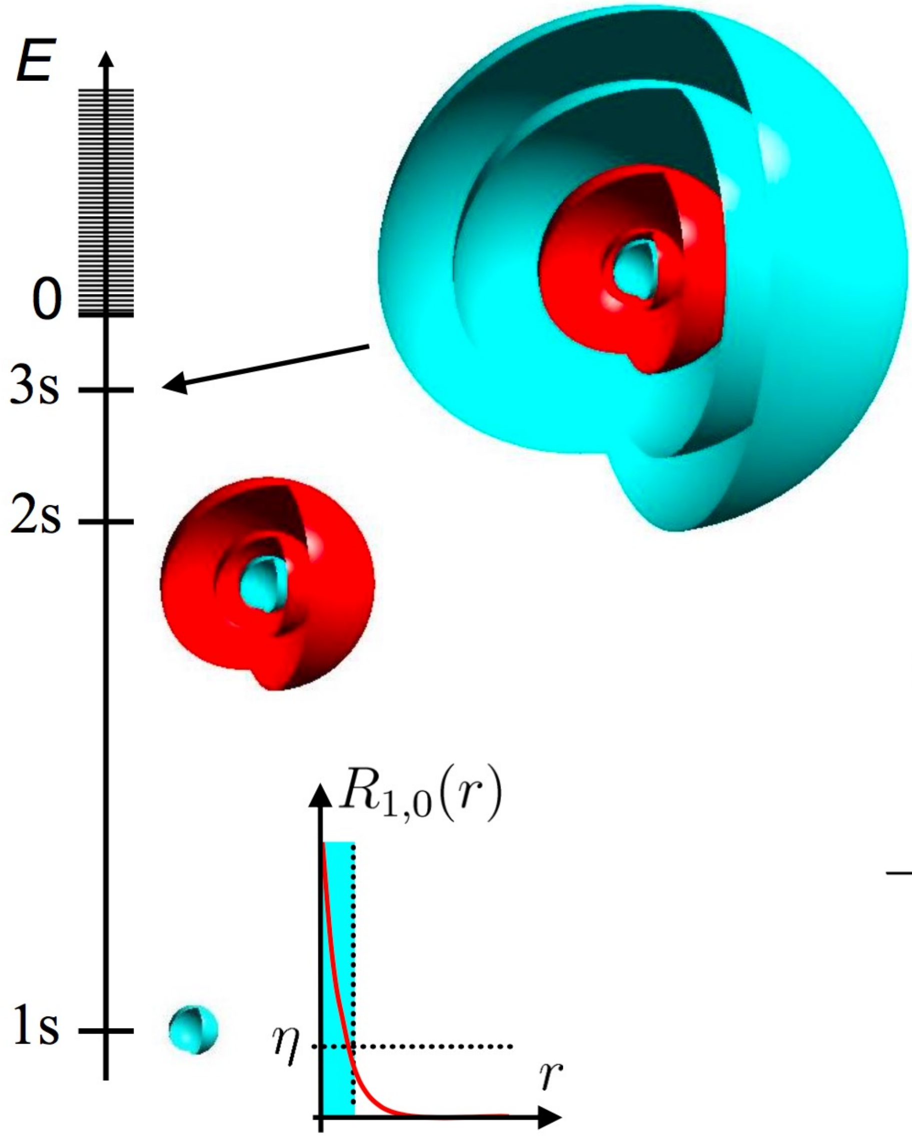
s-like atomic orbitals

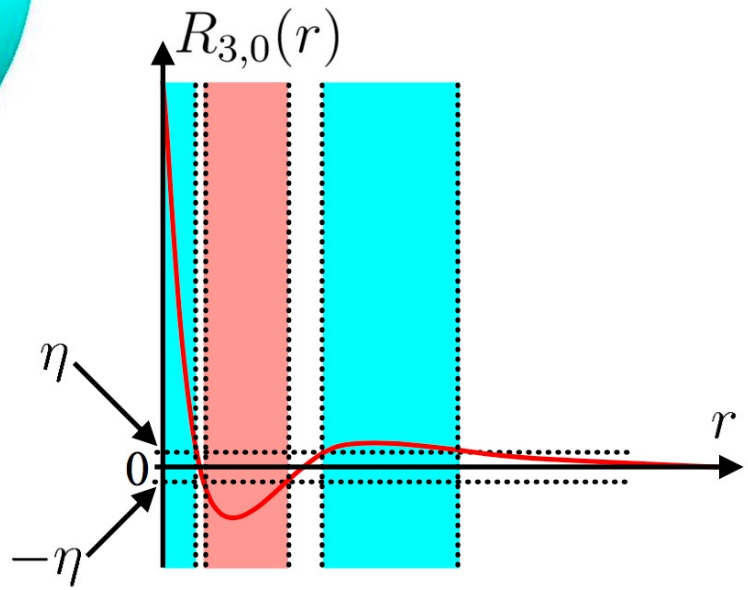
$n' = n - \ell - 1 = n - 1$



$$\psi_{n,0,0}(r,\theta,\varphi) = \frac{1}{\sqrt{4\pi}} R_{n,0}(r)$$

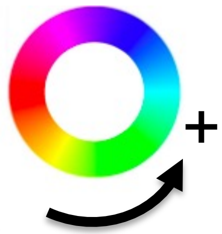
isodensity surface = spheres





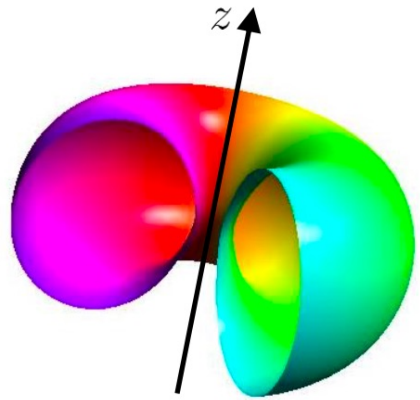
$$\ell = 1$$
$$n' = n - \ell - 1 = 0$$

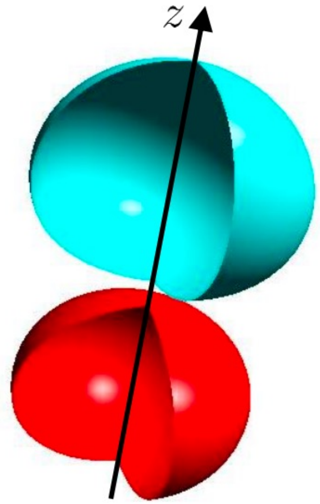
p-like atomic orbitals

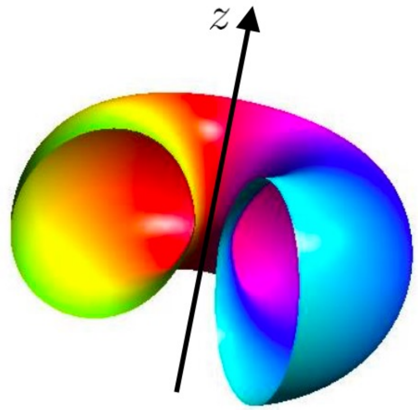


$$\psi_{2,1,m}(r,\theta,\varphi) = R_{2,1}(r) Y_{1,m}(\theta,\varphi) \qquad \text{avec} \qquad R_{2,1}(r) \propto r \exp\left(\frac{-r}{2a_1}\right)$$

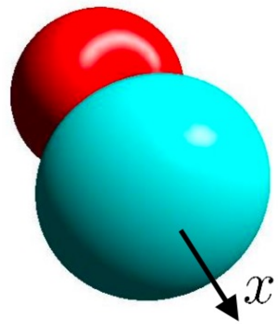
$$Y_{1,-1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\varphi} \qquad Y_{1,0}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta \qquad Y_{1,1}(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\varphi}$$







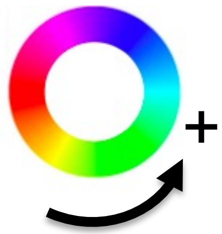
Note: $$\frac{-|2,1,1\rangle + |2,1,-1\rangle}{\sqrt{2}} = |2p_x\rangle$$



Reals orbitals, $2p_x$, $2p_y$, $2p_z$ used in chemistry

LCAO:
Linear Combination of Atomics Orbitals

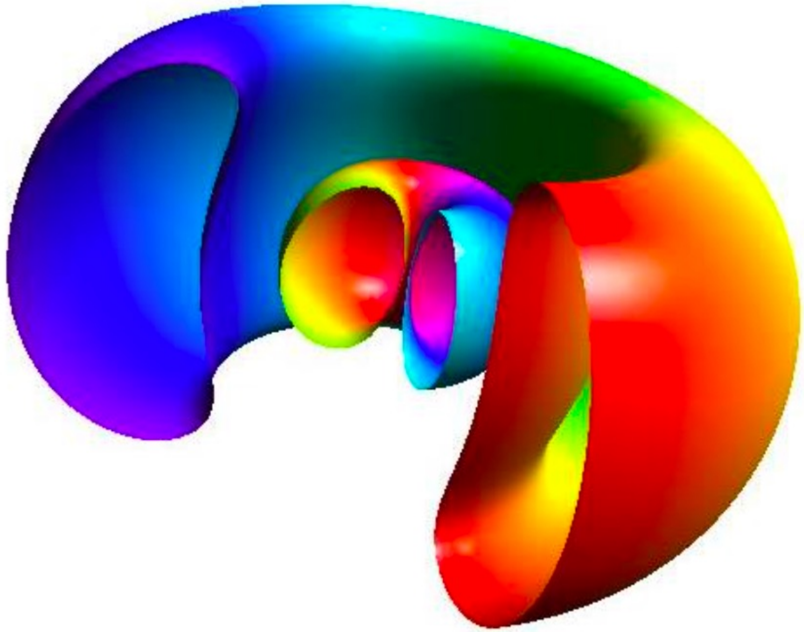
Quiz 10



A. $n = 3$
B. $n = 4$

C. $\ell = 0$
D. $\ell = 1$
E. $\ell = 2$

F. $m = -2$
G. $m = -1$
H. $m = 1$
I. $m = 2$



(n, ℓ, m) ?

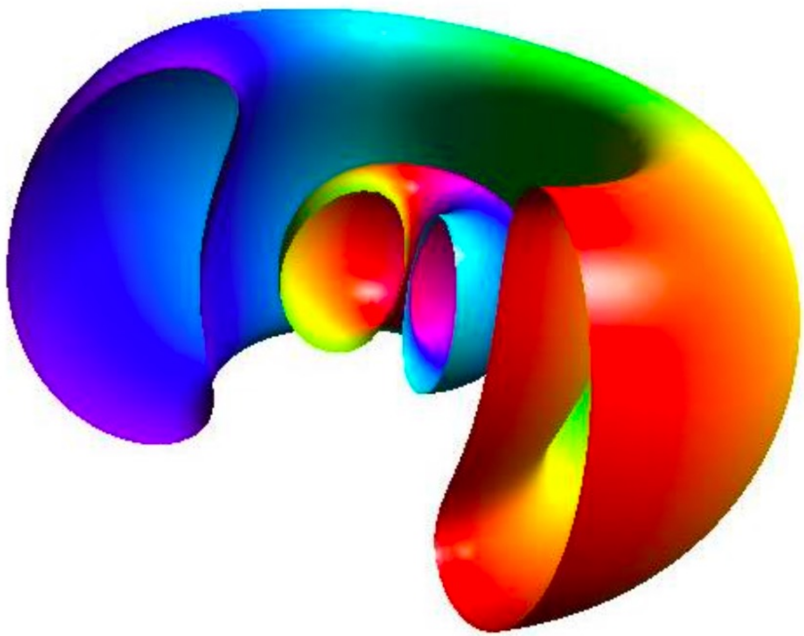
$$n = n' + \ell + 1$$

Quiz 10

A. $n = 3$
B. $n = 4$

C. $\ell = 0$
D. $\ell = 1$
E. $\ell = 2$

F. $m = -2$
G. $m = -1$
H. $m = 1$
I. $m = 2$



(n, ℓ, m) ?

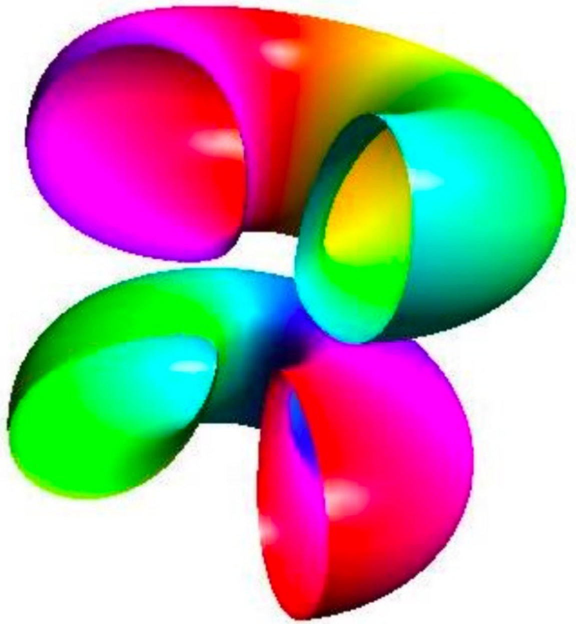
$$n = n' + \ell + 1$$

Quiz 11

A. $n = 3$
B. $n = 4$

C. $\ell = 0$
D. $\ell = 1$
E. $\ell = 2$

F. $m = -2$
G. $m = -1$
H. $m = 1$
I. $m = 2$



(n, ℓ, m) ?

$$n = n' + \ell + 1$$

Quiz 11

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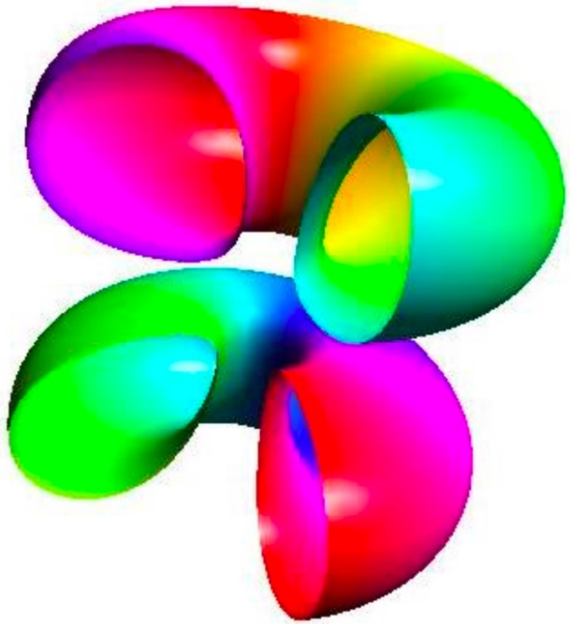
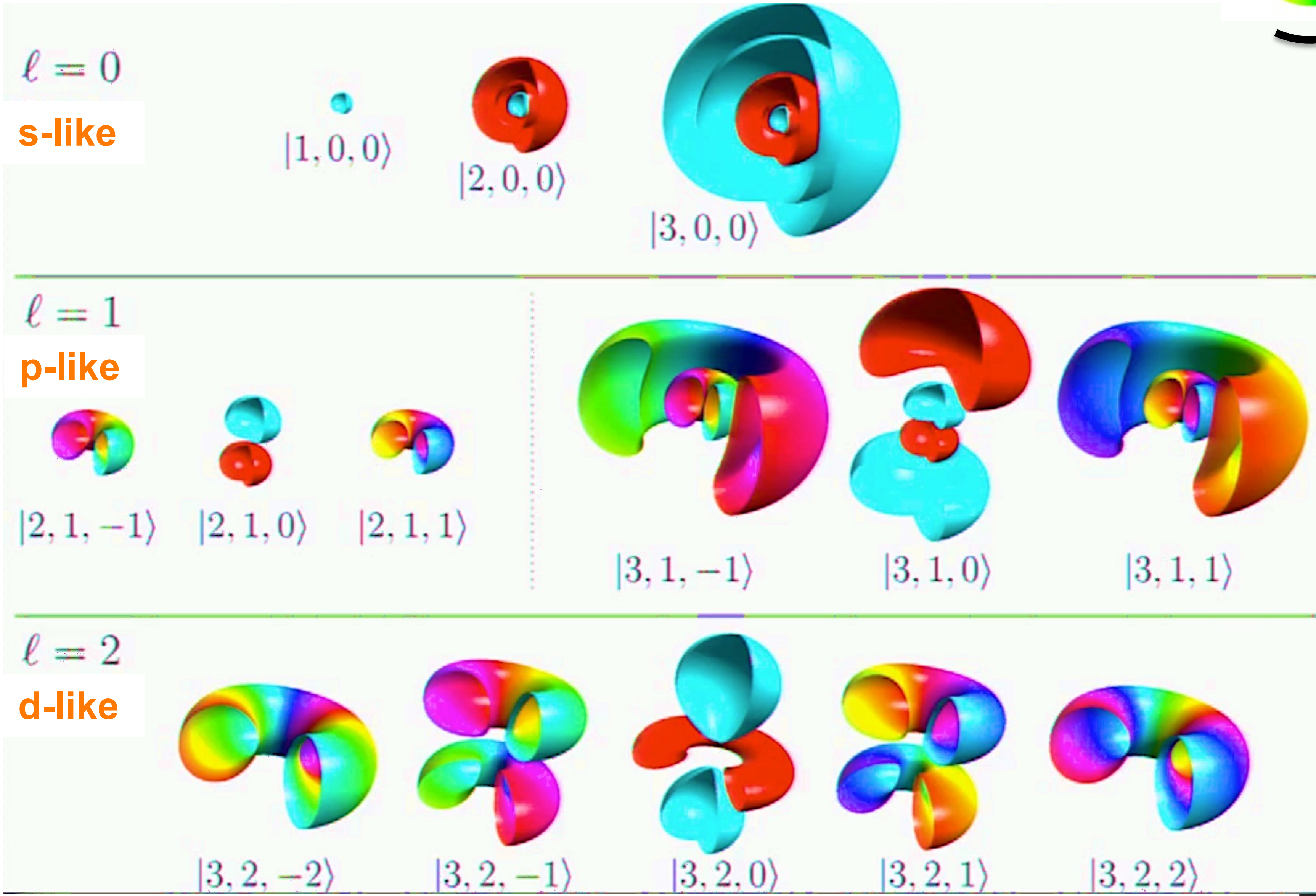


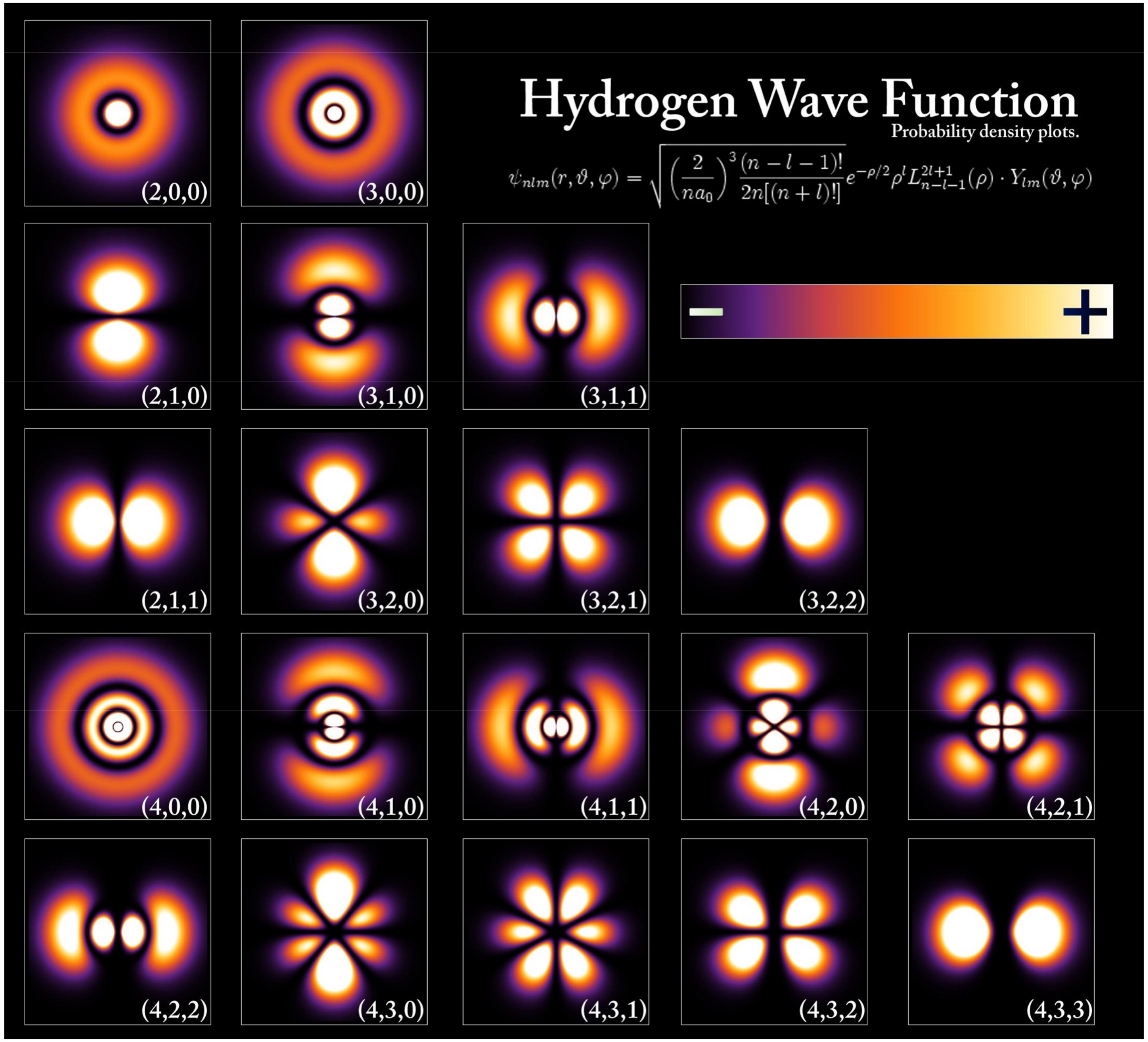
(n, ℓ, m) ?

$$n = n' + \ell + 1$$

Hydrogen atomic orbitals



Hydrogen atomic orbitals



4.
Time evolution

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle$$

Evolution of an eigenstate

$$\hat{H}|n,\ell,m\rangle = E_n|n,\ell,m\rangle = \hbar\omega_n|n,\ell,m\rangle$$

If $|\psi(0)\rangle = |n,\ell,m\rangle$ **then** $|\psi(t)\rangle = \exp(-i\omega_n t)|n,\ell,m\rangle$

$$\psi_{n,\ell,m}(r,\theta,\varphi) = R_{n,\ell}(r)Y_{\ell,m}(\theta,\varphi) = R_{n,\ell}(r)F_{\ell,m}(\theta)\exp(im\varphi)$$

$$\boxed{\psi(r,\theta,\varphi,t) = R_{n,\ell}(r)F_{\ell,m}(\theta)\exp\left(i(m\varphi-\omega_n t)\right)}$$

➡ $|\psi(r,\theta,\varphi,t)|^2$ **Time independent (stationary state)**

➡ **For** $m \neq 0$:

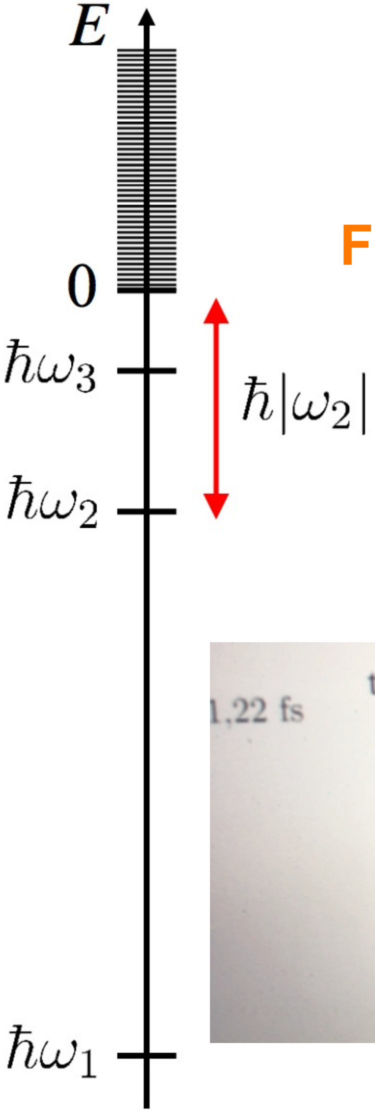
$$\psi(r,\theta,\varphi,t) = R_{n,\ell}(r)F_{\ell,m}(\theta)\exp\left(im\left(\varphi - \frac{\omega_n}{m}t\right)\right) = \psi\left(r,\theta,\varphi - \frac{\omega_n}{m}t, 0\right)$$

Rotation

Time evolution of l2,1,1>

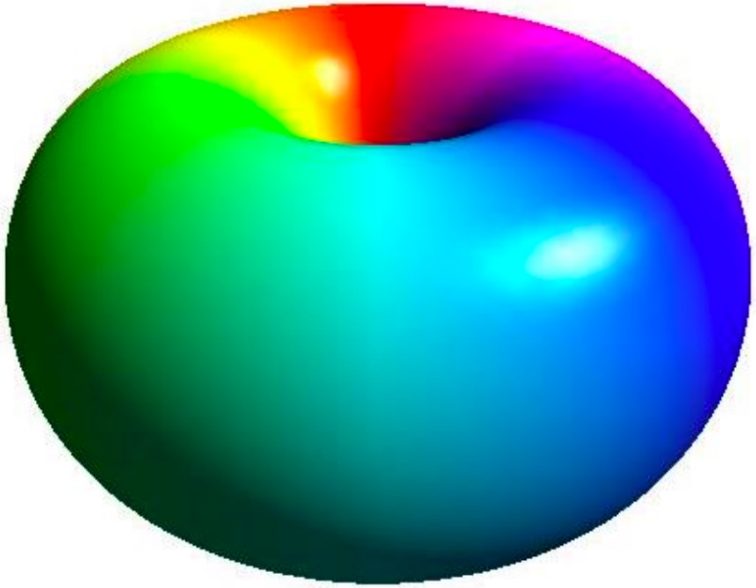
$$\psi(r,\theta,\varphi,t) = R_{n,\ell}(r)F_{\ell,m}(\theta)\exp\left(im\left(\varphi - \frac{\omega_n}{m}t\right)\right)$$

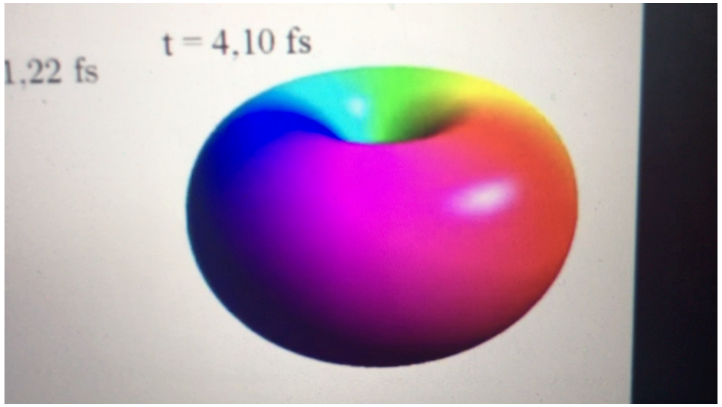
For instance $|\psi(0)\rangle = |2,1,1\rangle \qquad (n=2, \ell=1, m=1)$



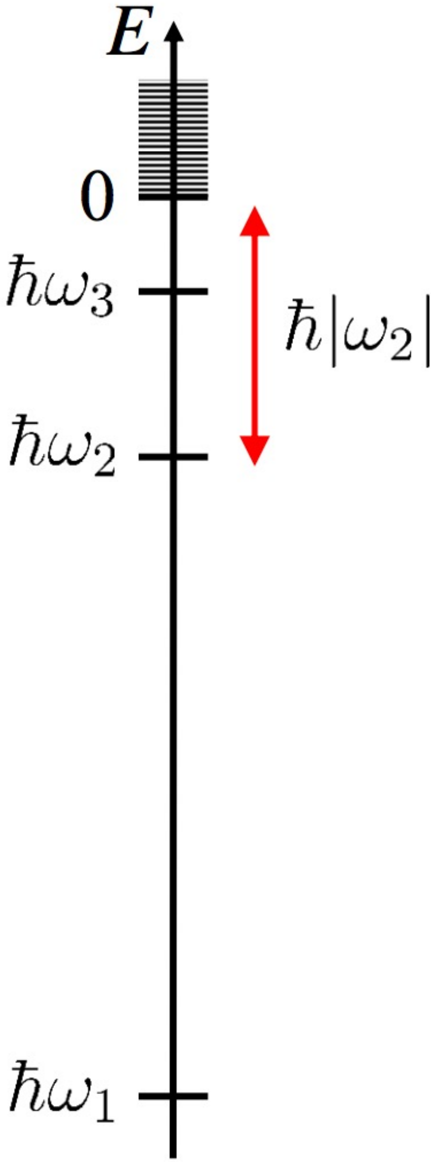
$$\frac{2\pi}{|\omega_2|} = 1{,}22 \text{ fs}$$

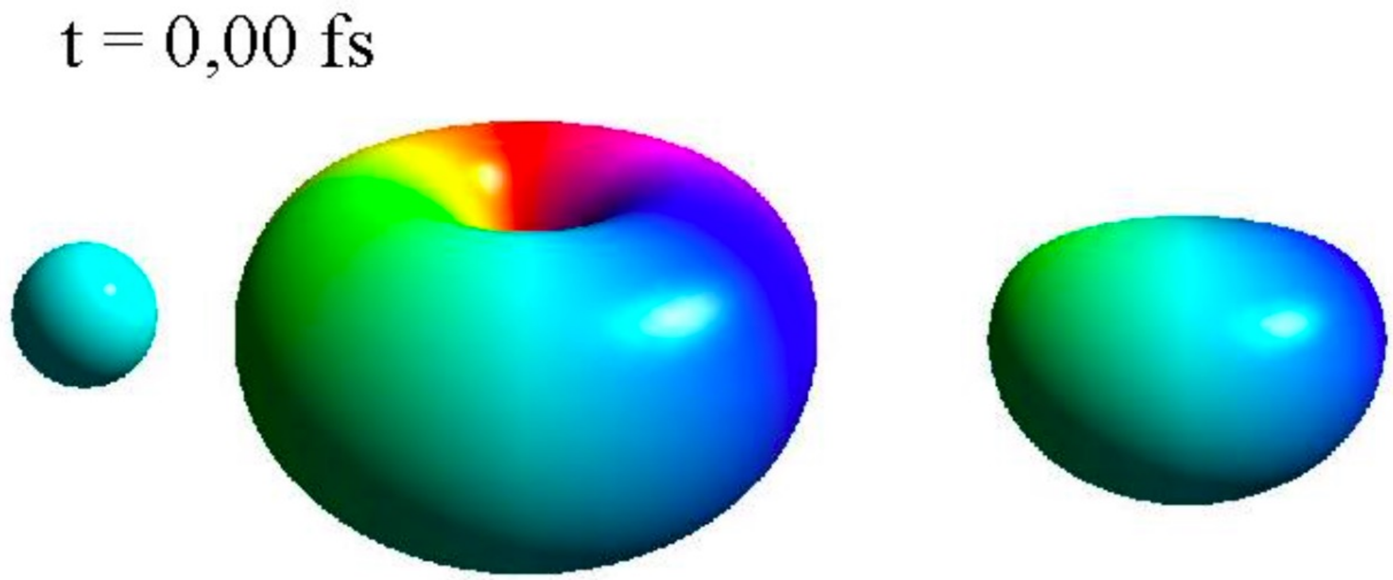
t = 0,00 fs





Time evolution of a linear superposition



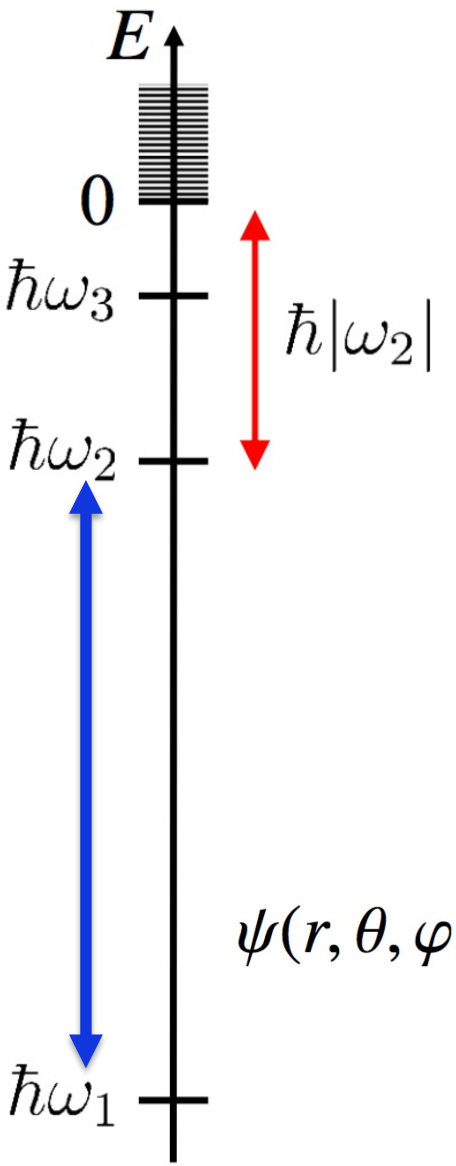


$$|\psi(0)\rangle = \frac{|100\rangle + \sqrt{3}|211\rangle}{2}$$

$$|\psi(t)\rangle = \frac{1}{2}[e^{-i\omega_1 t}\,|100\rangle + \sqrt{3}e^{-i\omega_2 t}\,|211\rangle]$$

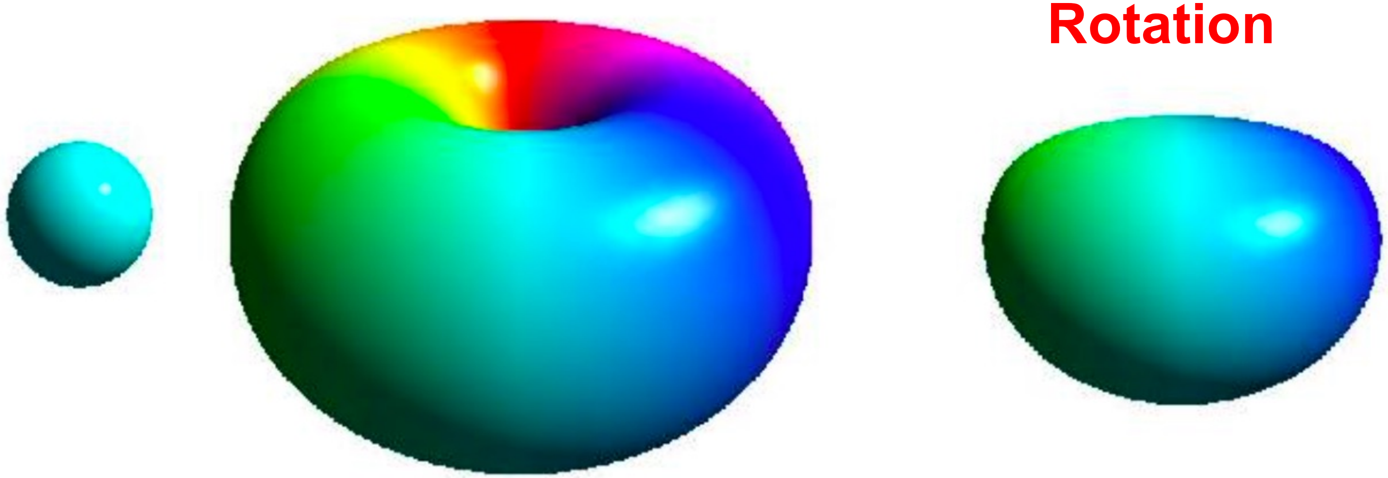
$$|\psi(t)\rangle = \frac{1}{2}e^{-i\omega_1 t}[|100\rangle + \sqrt{3}e^{-i(\omega_2-\omega_1)t}\,|211\rangle]$$

Time evolution of a linear superposition



t = 0,00 fs

Rotation

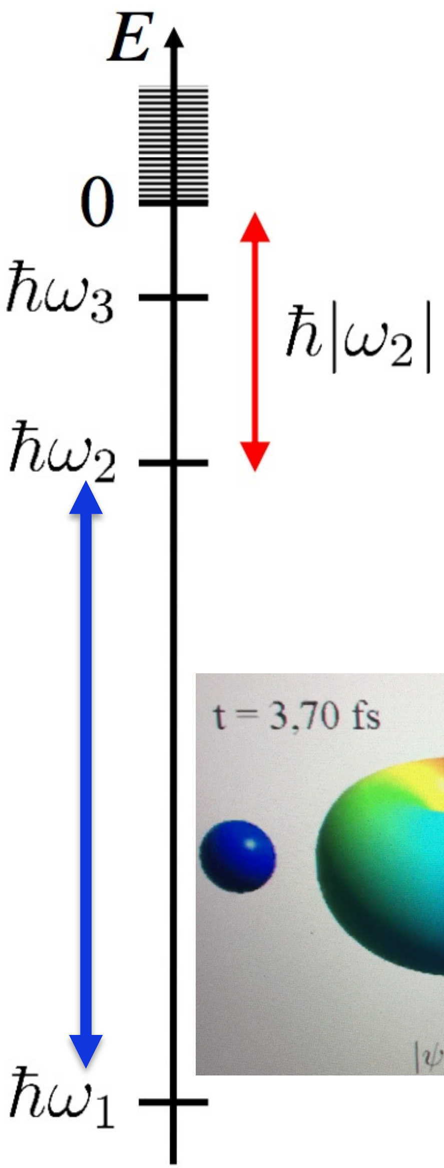


$$|\psi(0)\rangle = \frac{|100\rangle + \sqrt{3}|211\rangle}{2}$$

$$\psi(r,\theta,\varphi,t) = \frac{1}{2}e^{-i\omega_1 t}[R_{10}(r)F_{00}(\theta) + \sqrt{3}R_{21}(r)F_{11}(\theta)e^{i(\varphi-\omega_{21}t)}]$$

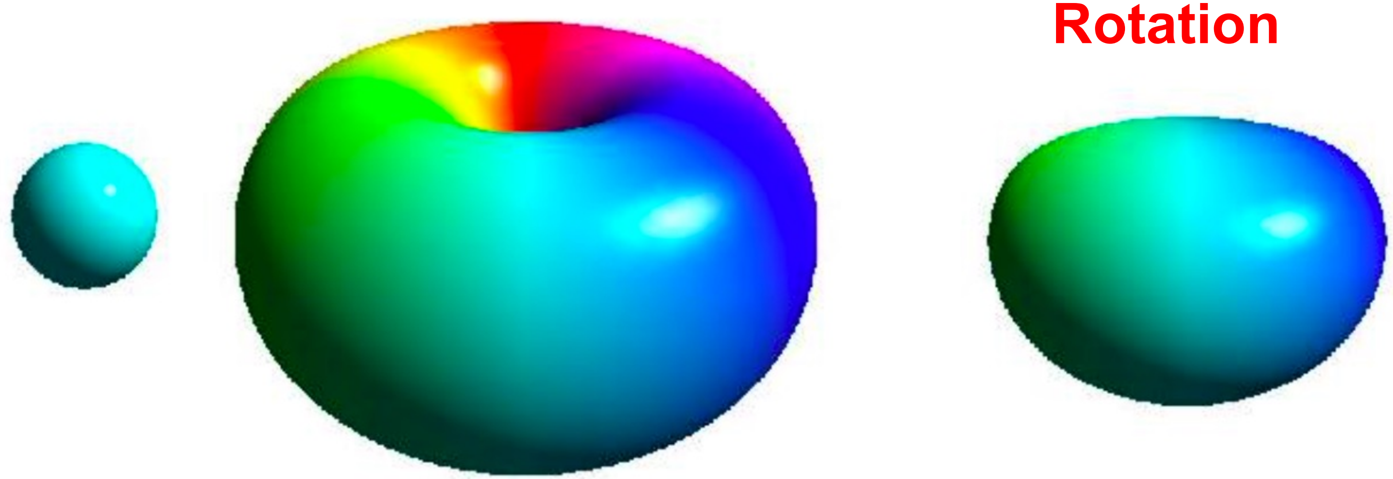
$$|\,\psi(r,\theta,\varphi,t)\,|^2 = f(r,\theta,\varphi-\omega_{21}t)$$

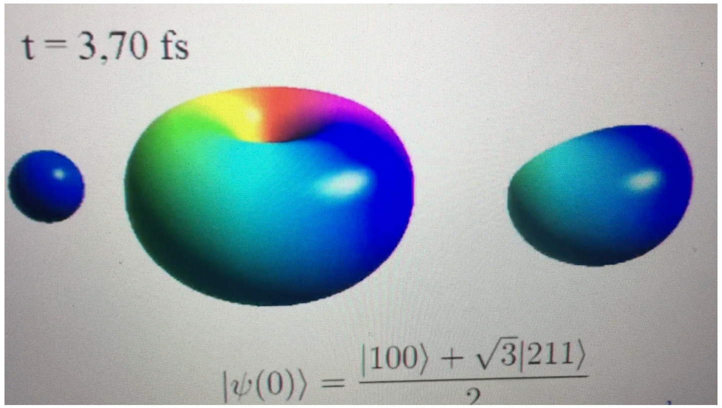
Time evolution of a linear superposition



t = 0,00 fs

Rotation

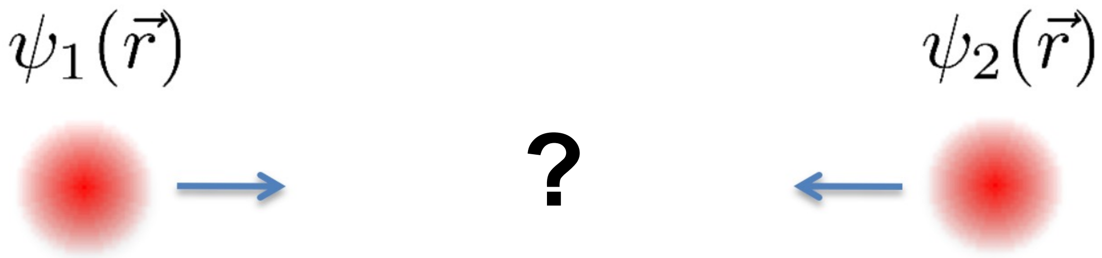




$$|\psi(0)\rangle = \frac{|100\rangle + \sqrt{3}|211\rangle}{2}$$

Section 10

Indistinguishable particles



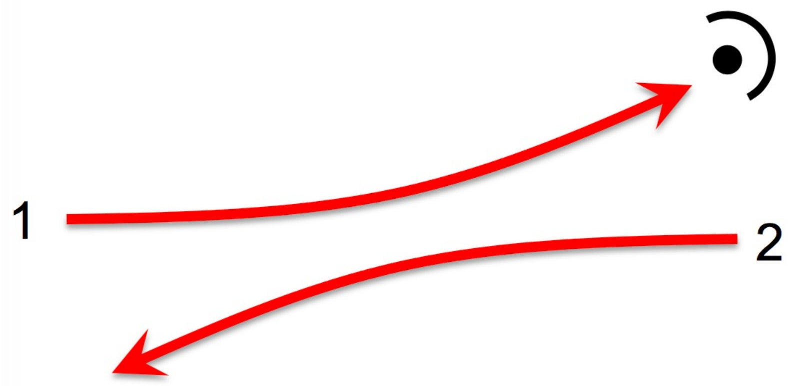
Identical particles

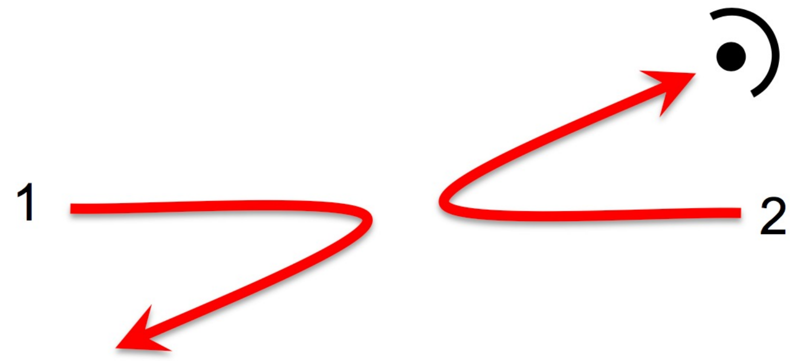
Two particles are indistinguishable or identical if their physical properties (mass, charge, etc.) are all identical

Example: 2 electrons or 2 protons

In classical physics, it is possible to track the trajectories of two identical particles. These particles are discernible

e.g. the two physical processes below are perfectly distinguishable



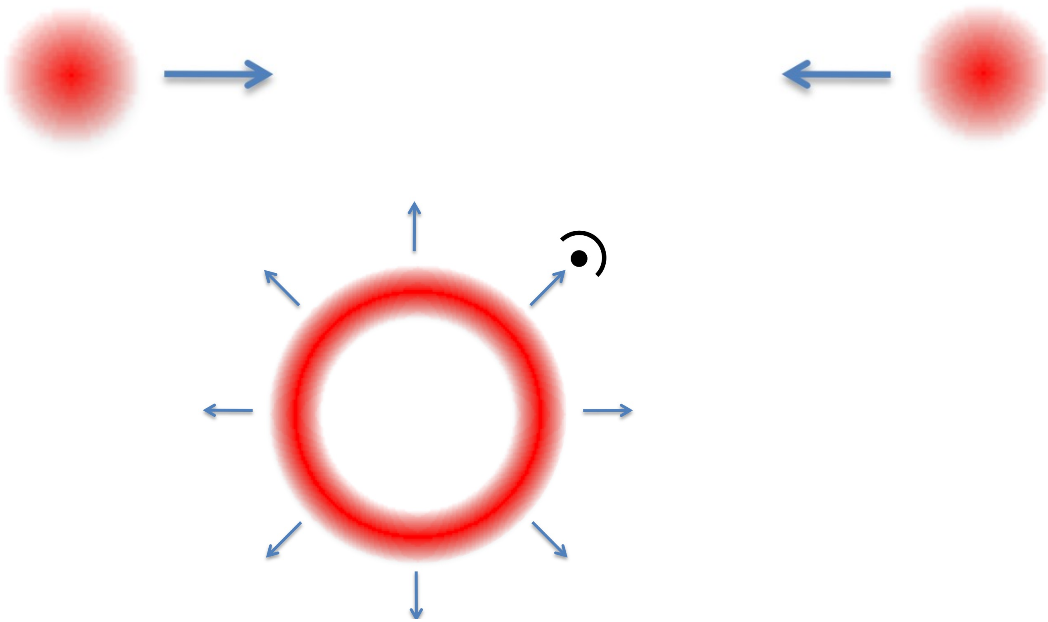


Identical particles

In quantum physics, the concept of trajectory does not exist anymore

Before collision

After collision



The question “which particle has been detected?” does not make sense in quantum physics since the particles are not discernable

How to describe the system?

$\psi_1(\vec{r})$ $\psi_2(\vec{r})$

$$\mathcal{E}_H = \mathcal{L}^2(\mathbb{R}^3) \otimes \mathcal{L}^2(\mathbb{R}^3)$$

Orbital

$$\psi(\vec{r}_a, \vec{r}_b) = \psi_1(\vec{r}_a)\psi_2(\vec{r}_b) \text{ ?}$$

or $\psi_2(\vec{r}_a)\psi_1(\vec{r}_b)$?

or $\lambda\psi_1(\vec{r}_a)\psi_2(\vec{r}_b) + \mu\psi_2(\vec{r}_a)\psi_1(\vec{r}_b)$?

What representation to describe the quantum system?

Exchange particles

$\hat{P}_{ab}$ is a permutation operator that acts by switching the labels on any two identical particles described by the joint position quantum state

$$\hat{P}_{ab}|a:\psi_1;b:\psi_2\rangle = |a:\psi_2;b:\psi_1\rangle$$ Fock states

Two particles w/o spin $\hat{P}_{ab}\Psi(\vec{r}_a,\vec{r}_b) = \Psi(\vec{r}_b,\vec{r}_a)$ $\mathcal{E}^{(a)}_{\text{externe}} \otimes \mathcal{E}^{(b)}_{\text{externe}}$

Two particles w/ spin $\mathcal{E}^{(a)}_{\text{externe}} \otimes \mathcal{E}^{(b)}_{\text{externe}} \otimes \mathcal{E}^{(a)}_{\text{spin}} \otimes \mathcal{E}^{(b)}_{\text{spin}} \leftarrow \mathcal{E}_H$

$$\hat{P}_{ab}|a:\psi_1;b:\psi_2\rangle \otimes |a:\sigma_1,b:\sigma_2\rangle = |a:\psi_2;b:\psi_1\rangle \otimes |a:\sigma_2,b:\sigma_1\rangle$$

$\hat{P}_{ab}$ is a Hermitian and unitary operator

$$\hat{P}^2_{ab} = \hat{I} \qquad \hat{P}^\dagger_{ab} = \hat{P}_{ab}$$

with eigenvalues of ± 1.

Exchange particles

$$|\Psi\rangle = \sum_{n,m} c_{n,m} |a:\psi_n\rangle \otimes |b:\psi_m\rangle$$

$$\hat{P}_{ab}|\Psi\rangle = \sum_{n,m} c_{n,m} |a:\psi_m\rangle \otimes |b:\psi_n\rangle = \sum_{m,n} c_{m,n} |a:\psi_n\rangle \otimes |b:\psi_m\rangle$$

Symmetric states $\hat{P}_{ab}|\Psi\rangle = |\Psi\rangle$ $c_{m,n} = c_{n,m}$

$$|\Psi\rangle = \sum_{n} c_{n,n} |a:\psi_n\rangle \otimes |b:\psi_n\rangle$$
$$+ \sum_{n<m} c_{n,m}\sqrt{2}\, \frac{|a:\psi_n\rangle \otimes |b:\psi_m\rangle + |a:\psi_m\rangle \otimes |b:\psi_n\rangle}{\sqrt{2}}$$

Antisymmetric states $\hat{P}_{ab}|\Psi\rangle = -|\Psi\rangle$ $c_{m,n} = -c_{n,m} \Rightarrow c_{n,n} = 0$

$$|\Psi\rangle = \sum_{n<m} c_{n,m}\sqrt{2}\, \frac{|a:\psi_n\rangle \otimes |b:\psi_m\rangle - |a:\psi_m\rangle \otimes |b:\psi_n\rangle}{\sqrt{2}}$$

Time evolution

The two particles are indistinguishable (invariance under the exchange of 2 particles as the rotational invariance seen in section 8)

$$\left[\hat{H},\hat{P}_{ab}\right]=0 \quad \text{and} \quad \left[\hat{U}(t,t_0),\hat{P}_{ab}\right]=0.$$

Consider $\hat{P}_{ab}|\Psi(t_0)\rangle = \epsilon|\Psi(t_0)\rangle$ avec $\epsilon = \pm 1$

$$\begin{aligned}
\hat{P}_{ab}|\Psi(t)\rangle &= \hat{P}_{ab}\hat{U}(t,t_0)|\Psi(t_0)\rangle \\
&= \hat{U}(t,t_0)\hat{P}_{ab}|\Psi(t_0)\rangle \\
&= \hat{U}(t,t_0)\epsilon|\Psi(t_0)\rangle \\
&= \epsilon|\Psi(t)\rangle
\end{aligned}$$

A symmetric (antisymmetric) state remains symmetric (antisymmetric).
However, quantum physics allows principle of superposition. Can we put the system in a linear superposition of symmetric and antisymmetric states? Another postulate is required at this stage.

Pauli exclusion principle

It is a postulate of symmetrization introduced by Pauli

All particles in Nature are Bosons or Fermions

Bosons: The state vector is always symmetric under particle exchange

$$\hat{P}_{ab}|\Psi\rangle = |\Psi\rangle$$

Fermions: The state vector is always antisymmetric under particle exchange

$$\hat{P}_{ab}|\Psi\rangle = -|\Psi\rangle$$

Read also P. A. M. Dirac, « On the theory of quantum mechanics », Proceedings on the Royal Society A, Vol. 112, pp. 661, 1926

Spin-statistic theorem

The spin–statistic theorem relates the intrinsic spin of a particle (angular momentum not due to the orbital motion) to the particle statistics it obeys

The demonstration of this theorem requires the quantum field theory that is beyond the scope of this lecture. In our case, use it as a postulate

→ Particles with integer spin (photons, phonons, mesons pi, etc.) can only be found in symmetric states hence these particles are bosons.
Bose-Einstein statistics

→ Particles with half-integer spin (electrons, protons, neutrons, etc.) can only be found in antisymmetric states – these particles are fermions.
Fermi-Dirac statistics

Composite particles

The spin-statistics theorem remains valid for any composite particles

Composite particles with total spin equal to one half plus an integer are also fermions. Conveniently, because spin only comes in units of one half, this means any composite particle which contains an odd number of fermions is a fermion

→ Proton or neutron (3 quarks): s=1/2 [Fermion]

→ Alpha-particle (2 protons and 2 neutrons) : s=0 [Boson]

Exercise: can you guess whether these two isotopes of sodium are fermions or bosons?

1. ${}^{22}_{11}\mathrm{Na}$ A = 22, Z = 11
2. ${}^{23}_{11}\mathrm{Na}$ A = 23, Z = 11

?

Composite particles

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Exercise: can you guess whether these two isotopes of sodium are fermions or bosons?

Z protons
Z electrons
A-Z neutrons

1. $^{22}_{11}\mathrm{Na}$	A = 22, Z = 11	Fermion
2. $^{23}_{11}\mathrm{Na}$	A = 23, Z = 11	Boson

Composite particles

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Exercise: And assuming the two nuclei?

Z protons
Z electrons
A-Z neutrons

1. ${}^{22}_{11}\mathrm{Na}$ — A = 22, Z = 11
2. ${}^{23}_{11}\mathrm{Na}$ — A = 23, Z = 11

Composite particles

The spin-statistics theorem remains valid for any composite particles

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→ Alpha-particle (2 protons and 2 neutrons) : s=0 [Boson]

Exercise: And considering the two nuclei?

Z protons
Z electrons
A-Z neutrons

1. ${}^{22}_{11}\mathrm{Na}$	A = 22, Z = 11	Boson
2. ${}^{23}_{11}\mathrm{Na}$	A = 23, Z = 11	Fermion

Composite particles

PARTICLE	SYMBOL	CHARGE	MASS	SPIN	STATISTICS	DECAY SCHEME	LIFETIME (SECONDS)
NEUTRINO	υ	0	0	1/2	FERMI-DIRAC	STABLE	
ELECTRON	e	–	1	1/2	FERMI-DIRAC	STABLE	
POSITRON	p	+	1	1/2	FERMI-DIRAC	STABLE	
POSITIVE MU MESON	μ^+	+	210	1/2	FERMI-DIRAC	$\mu^+ \rightarrow p + 2\upsilon$	2.1×10^{-6}
NEGATIVE MU MESON	μ^-	–	210	1/2	FERMI-DIRAC	$\mu^- \rightarrow e + 2\upsilon$	2.1×10^{-6}
KAPPA MESON	κ	+	1200 ?	1/2 ?	FERMI-DIRAC ?	$\kappa \rightarrow \mu^+ + (?)\, 2\upsilon$	10^{-10} ?
PROTON	P	+	1836	1/2	FERMI-DIRAC	STABLE	
ANTIPROTON ?	$\overline{P}$	–	1836	1/2	FERMI-DIRAC	STABLE	
NEUTRON	N	0	1838.5	1/2	FERMI-DIRAC	$N \rightarrow P + e + \upsilon$	750
ANTINEUTRON ?	$\overline{N}$	0	1838.5	1/2	FERMI-DIRAC	$\overline{N} \rightarrow \overline{P} + p + \upsilon$	750
POSITIVE V-PARTICLE	V^+	+	2600 ?	?	FERMI-DIRAC ?	$V^+ \rightarrow N + \pi^+ + (?)\, \pi^0$	10^{-13} ?
NEGATIVE V-PARTICLE	V^-	–	2600 ?	?	FERMI-DIRAC ?	$V^- \rightarrow N + \pi^- + (?)\, \pi^0$	10^{-13} ?
NEUTRAL V-PARTICLE	V^0	0	2600 ?	?	FERMI-DIRAC ?	$V^0 \rightarrow N + \pi^+ + \pi^-$? $V^0 \rightarrow P + \pi^- + (?)\, \pi^0$	3×10^{-10}
PHOTON	γ	0	0	1	BOSE-EINSTEIN	STABLE	
GRAVITON	G	0	0	2	BOSE-EINSTEIN	STABLE	
POSITIVE PI MESON	π^+	+	276	0	BOSE-EINSTEIN	$\pi^+ \rightarrow \mu^+ + \upsilon$	2.6×10^{-8}
NEGATIVE PI MESON	π^-	–	276	0	BOSE-EINSTEIN	$\pi^- \rightarrow \mu^- + \upsilon$	2.6×10^{-8}
NEUTRAL PI MESON	π^0	0	265	0	BOSE-EINSTEIN	$\pi^0 \rightarrow 2\gamma$	10^{-14}
TAU MESON	τ	+ or –	966	0 ?	BOSE-EINSTEIN	$\tau \rightarrow 3\pi$	10^{-9} ?

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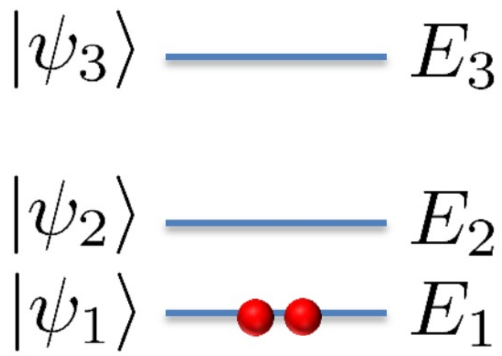
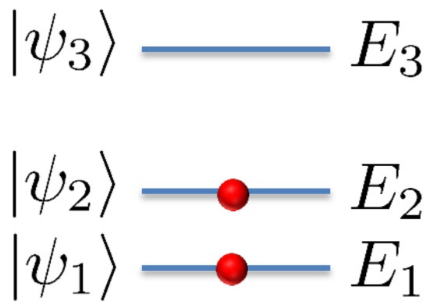
2 identical bosons with spin 0

Ground state level ($E=2E_1$)



$$|\Psi\rangle = |a:\psi_1\rangle \otimes |b:\psi_1\rangle$$

First excited state ($E=E_1+E_2$)



$$|\Psi\rangle = \frac{|a:\psi_1\rangle \otimes |b:\psi_2\rangle + |a:\psi_2\rangle \otimes |b:\psi_1\rangle}{\sqrt{2}}$$

Dimension of the Hilbert space associated to the energy E_2+E_1 is reduced from 2 to 1 (identical particles)

System with two spin-½

$$\mathcal{E}_H = \mathcal{E}_{\text{spin}}^{(a)} \otimes \mathcal{E}_{\text{spin}}^{(b)}$$

$$\dim \mathcal{E}_{\text{spin}}^{(a)} = \dim \mathcal{E}_{\text{spin}}^{(b)} = 2 \qquad \dim \mathcal{E}_H = 2 \times 2 = 4$$

One electron and one proton in the Hydrogen atom

$$\{|e:+\rangle \otimes |p:+\rangle, |e:+\rangle \otimes |p:-\rangle, |e:-\rangle \otimes |p:+\rangle, |e:-\rangle \otimes |p:-\rangle\}$$

Two protons in the Hydrogen molecule

$$\{|a:+\rangle \otimes |b:+\rangle, |a:+\rangle \otimes |b:-\rangle, |a:-\rangle \otimes |b:+\rangle, |a:-\rangle \otimes |b:-\rangle\}$$

Any virtual system with two spin-1/2 (two state level systems) → Photon pair (clockwise/anti-clockwise circularly and linearly polarized)

$$\{|a:\sigma_+\rangle \otimes |b:\sigma_+\rangle, |a:\sigma_+\rangle \otimes |b:\sigma_-\rangle, |a:\sigma_-\rangle \otimes |b:\sigma_+\rangle, |a:\sigma_-\rangle \otimes |b:\sigma_-\rangle\}$$

$$\{|a:\updownarrow\rangle \otimes |b:\updownarrow\rangle, |a:\updownarrow\rangle \otimes |b:\leftrightarrow\rangle, |a:\leftrightarrow\rangle \otimes |b:\updownarrow\rangle, |a:\leftrightarrow\rangle \otimes |b:\leftrightarrow\rangle\}$$

2 particles with spin-½

Coupling two particles with spin ½ means that the total angular momentum is integer and only equals s=0 or s=1 (not demonstrated in this course)

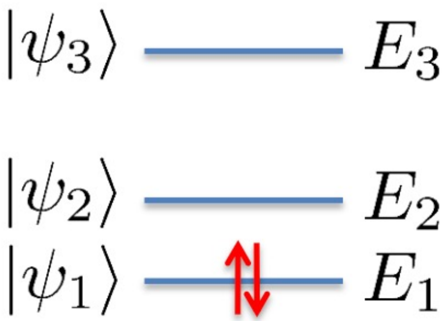
$$\mathcal{E}_{\text{spin}^{1/2}} \otimes \mathcal{E}_{\text{spin}^{1/2}} = \mathcal{E}_{s=1} \oplus \mathcal{E}_{s=0}$$

$$\Longleftrightarrow \qquad \boxed{2 \times 2 = 3 + 1}$$

Spin ½   Spin ½   **spin 1 (triplet)**   **spin 0 (singlet)**

2 identical fermions with spin-½

Ground state level ($E=2E_1$)



$$\mathcal{E}_H = \mathcal{E}^{(a)}_{\text{externe}} \otimes \mathcal{E}^{(a)}_{\text{spin}} \otimes \mathcal{E}^{(b)}_{\text{externe}} \otimes \mathcal{E}^{(b)}_{\text{spin}}$$

$$= \underbrace{\mathcal{E}^{(a)}_{\text{externe}} \otimes \mathcal{E}^{(b)}_{\text{externe}}}_{\text{Orbital}} \otimes \underbrace{\mathcal{E}^{(a)}_{\text{spin}} \otimes \mathcal{E}^{(b)}_{\text{spin}}}_{\text{spin}}$$

$$|\Psi\rangle = |a:\psi_1\rangle \otimes |b:\psi_1\rangle \otimes \left(c_{++}|a:+,b:+\rangle + c_{+-}|a:+,b:-\rangle \right.$$
$$\left. + c_{-+}|a:-,b:+\rangle + c_{--}|a:-,b:-\rangle\right)$$

dim=4

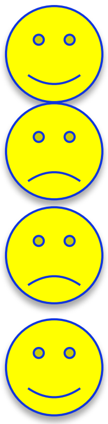
$$\hat{P}_{ab}|\Psi\rangle = -|\Psi\rangle \;\Rightarrow c_{++} = c_{--} = 0 \;\text{ et }\; c_{+-} = -c_{-+}$$

$$|\Psi\rangle = \underbrace{|a:\psi_1\rangle \otimes |b:\psi_1\rangle}_{\substack{\text{Orbital} \\ \text{(symmetric)}}} \otimes \underbrace{\frac{|a:+,b:-\rangle - |a:-,b:+\rangle}{\sqrt{2}}}_{\substack{\text{spin (singlet state)} \\ \text{(antisymmetric)}}}$$

dim=1

2 identical fermions with spin-½

First excited state level ($E=E_1+E_2$)



$$(|a:\psi_1\rangle \otimes |b:\psi_2\rangle + |a:\psi_2\rangle \otimes |b:\psi_1\rangle)/\sqrt{2} \otimes |s=0, m=0\rangle$$

$$(|a:\psi_1\rangle \otimes |b:\psi_2\rangle - |a:\psi_2\rangle \otimes |b:\psi_1\rangle)/\sqrt{2} \otimes |s=0, m=0\rangle$$

$$(|a:\psi_1\rangle \otimes |b:\psi_2\rangle + |a:\psi_2\rangle \otimes |b:\psi_1\rangle)/\sqrt{2} \otimes |s=1, m\rangle$$

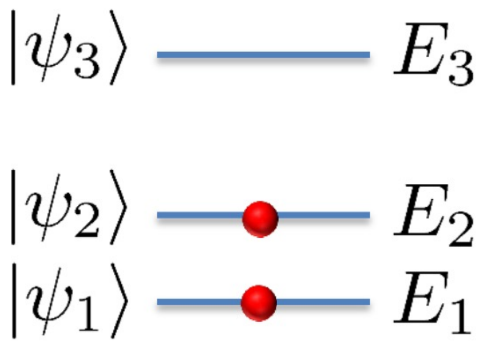
$$(|a:\psi_1\rangle \otimes |b:\psi_2\rangle - |a:\psi_2\rangle \otimes |b:\psi_1\rangle)/\sqrt{2} \otimes |s=1, m\rangle$$

$$|s=0, m=0\rangle = (|+-\rangle - |-+\rangle)/\sqrt{2}$$

$$\boxed{\begin{aligned} &|s=1, m=1\rangle = |++\rangle \\ &|s=1, m=0\rangle = (|+-\rangle + |-+\rangle)/\sqrt{2} \\ &|s=1, m=-1\rangle = |--\rangle \end{aligned}}$$

spin (triplet state) symmetric

dim=8 $\downarrow$ dim=4



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Generalization to N particles

Many-body interaction has to be taken into account in the Hamiltonian

$$\hat{H} = \sum_{n=1}^{Z} \frac{\hat{p}_n^2}{2m_e} - \sum_{n=1}^{Z} \frac{Ze^2}{\hat{r}_n} + \underbrace{\sum_{n=1}^{Z} \sum_{m=n+1}^{Z} \frac{e^2}{|\hat{\vec{r}}_n - \hat{\vec{r}}_m|}}_{\text{Coulomb interaction between electrons}}$$

Many situations in physics and chemistry involve N identical particles like atoms with Z electrons

Physics of semiconductors devices also requires the inclusion of many body interaction

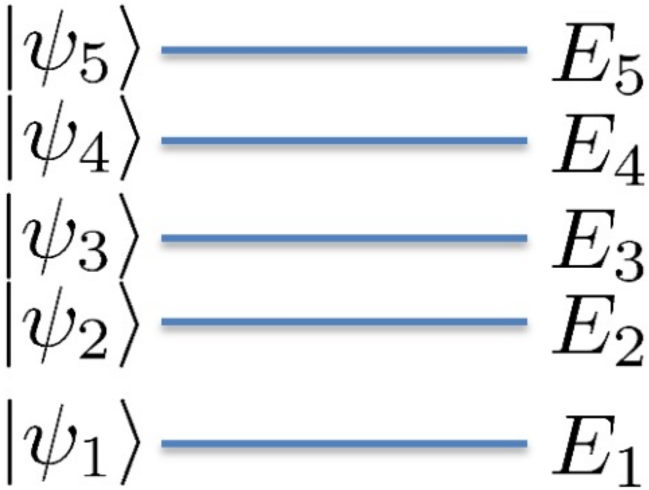
Generalization to N particles

We do not consider the interaction between particles

$$\hat{H} = \sum_{n=1}^{N} \hat{I}^{(1)} \otimes \ldots \otimes \hat{h}^{(n)} \otimes \ldots \otimes \hat{I}^{(N)} = \sum_{n=1}^{N} \hat{h}^{(n)}$$

We also assume that the eigenstates and eigenvalues of one particle are known

$$\hat{h}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$$



$$|\Psi\rangle = |1:\psi_{\alpha_1}\rangle \otimes |2:\psi_{\alpha_2}\rangle \otimes \ldots \otimes |N:\psi_{\alpha_N}\rangle$$ **Eigenvector of** $\hat{H}$

$$E = E_{\alpha_1} + E_{\alpha_2} + \ldots + E_{\alpha_N}$$ **Eigenvalues of** $\hat{H}$

System of N bosons

Consider N! p-permutations of {1,2,..,N} as well as the corresponding operators P_p acting in the Hilbert space

→ The state vector must be invariant whatever the permutations

Consider the given configuration

$$|1:\psi_{\alpha_1}\rangle \otimes |2:\psi_{\alpha_2}\rangle \otimes \ldots \otimes |N:\psi_{\alpha_N}\rangle$$

Using the postulate of symmetrization, the state vector becomes

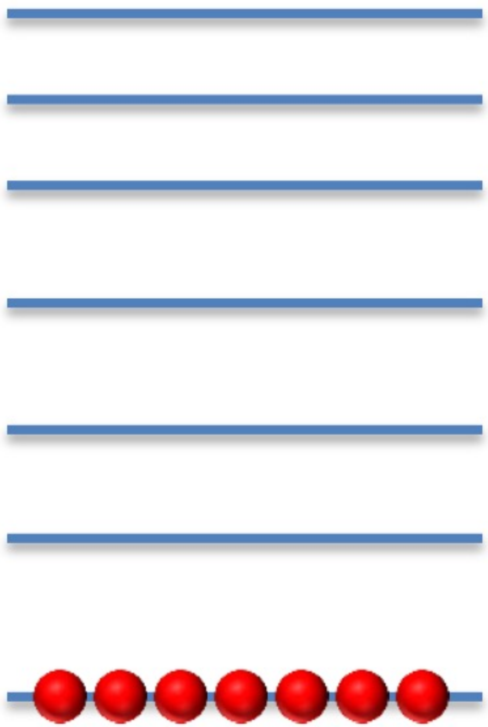
$$|\Psi\rangle = \frac{C}{\sqrt{N!}} \sum_p \hat{P}_p |1:\psi_{\alpha_1}\rangle \otimes \ldots \otimes |N:\psi_{\alpha_N}\rangle$$

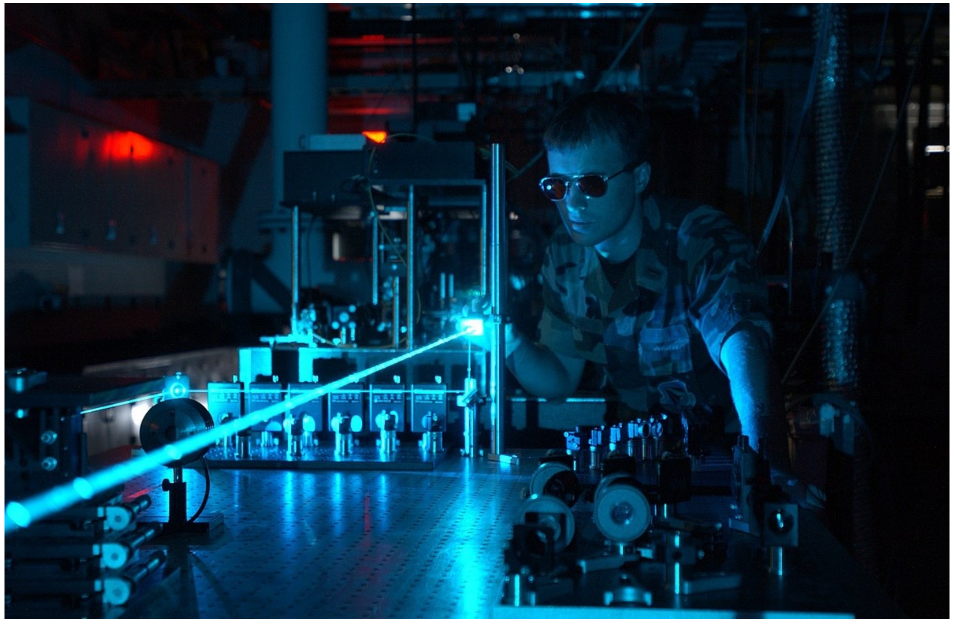
$$\hat{P}_p |\Psi\rangle = |\Psi\rangle$$

and C is a normalization constant

System of N bosons

$$|\Psi\rangle = |1 : \psi_1\rangle \otimes |2 : \psi_1\rangle \otimes \ldots \otimes |N : \psi_1\rangle$$





$$E_0 = N\epsilon_1$$

N bosons can be stacked in the same state → LASER

System of N fermions

Pauli exclusion principle : $\hat{P}_p\,|\Psi\rangle = \epsilon_p\,|\Psi\rangle$

$$|1:\psi_{\alpha_1}\rangle \otimes |2:\psi_{\alpha_2}\rangle \otimes \ldots \otimes |N:\psi_{\alpha_N}\rangle$$

Signature of the Permutation

Using anti-symmetrization, we get the following state vector

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \sum_p \epsilon_p \hat{P}_p |1:\psi_{\alpha_1}\rangle \otimes \ldots \otimes |N:\psi_{\alpha_N}\rangle$$

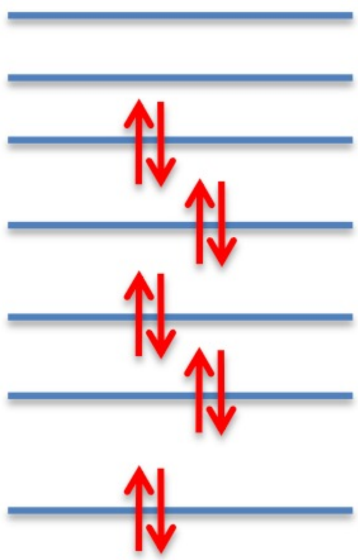
$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |1:\psi_{\alpha_1}\rangle & |1:\psi_{\alpha_2}\rangle & \ldots & |1:\psi_{\alpha_N}\rangle \\ |2:\psi_{\alpha_1}\rangle & |2:\psi_{\alpha_2}\rangle & \ldots & |2:\psi_{\alpha_N}\rangle \\ \vdots & \vdots & & \vdots \\ |N:\psi_{\alpha_1}\rangle & |N:\psi_{\alpha_2}\rangle & \ldots & |N:\psi_{\alpha_N}\rangle \end{vmatrix}$$

Slater determinant

→ vanishes when two columns are identical e.g two or more identical fermions cannot occupy the same state (Pauli)

System of N fermions with s=1/2

Useful to explain the construction of the atomic and molecular orbitals, the energy bands in solids, and of course the stability of matter



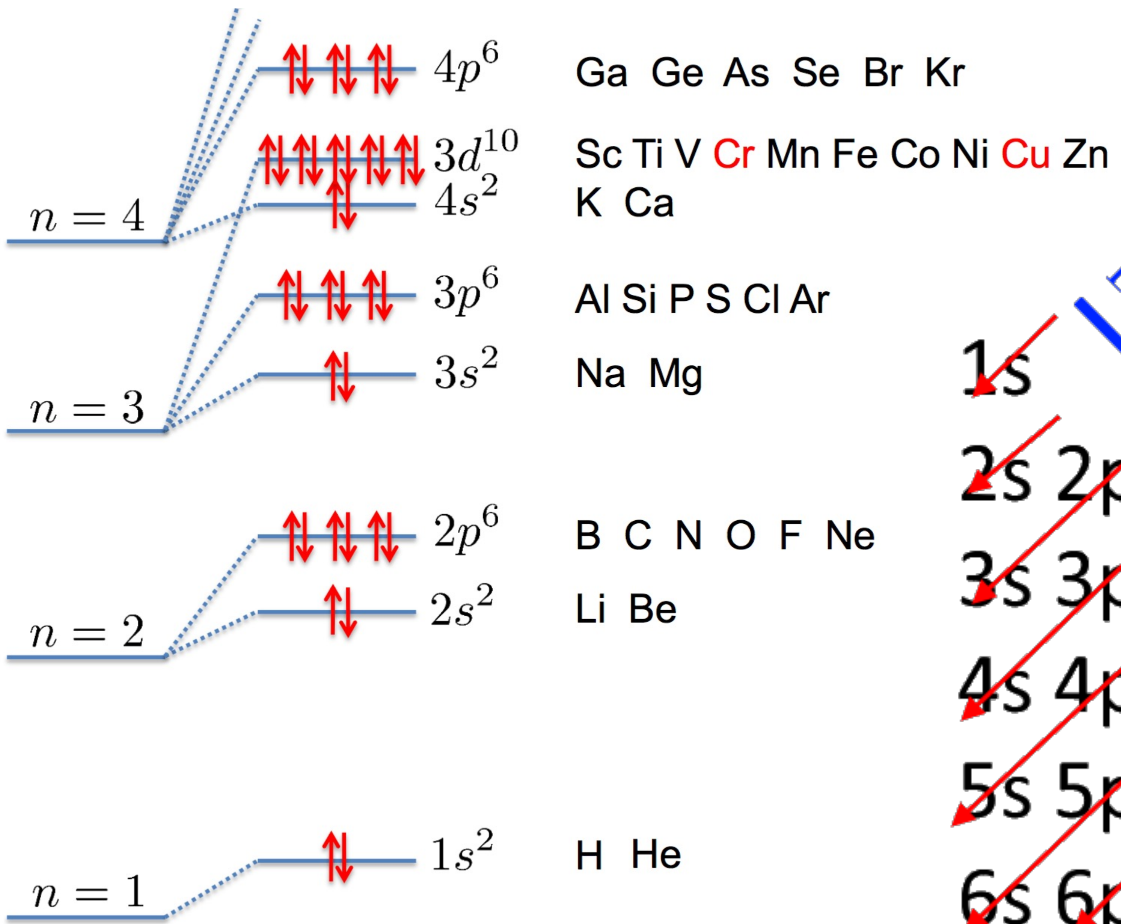
$$E_0 = \sum_{i=1}^{N} \epsilon_i$$

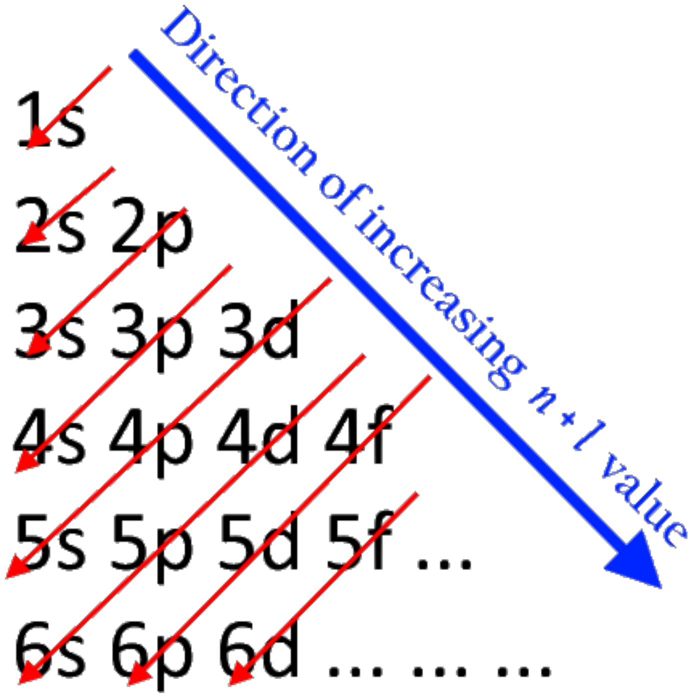
$$\hat{h}|\psi_\alpha \pm\rangle = E_\alpha |\psi_\alpha \pm\rangle$$

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |1:\psi_1+\rangle & |1:\psi_1-\rangle & |1:\psi_2+\rangle & \dots & |1:\psi_{N/2}-\rangle \\ |2:\psi_1+\rangle & |2:\psi_1-\rangle & |2:\psi_2+\rangle & \dots & |2:\psi_{N/2}-\rangle \\ \vdots & \vdots & \vdots & & \vdots \\ |N:\psi_1+\rangle & |N:\psi_1-\rangle & |N:\psi_2+\rangle & \dots & |N:\psi_{N/2}-\rangle \end{vmatrix}$$

Aufbau principle

In an atom or ion, electrons fill atomic orbitals of the lowest available energy levels before occupying higher levels leading to the most stable electron configuration possible wavefunctions





Periodic table

$$1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,[4s^2\,3d^{10}]\,4p^6\,[5s^2\,4d^{10}]\,5p^6\,[6s^2\,4f^{14}\,5d^{10}]\,6p^6\,[7s^2\,5f^{14}]$$

$\ell = 1$

Transition metals $(\ell = 2)$

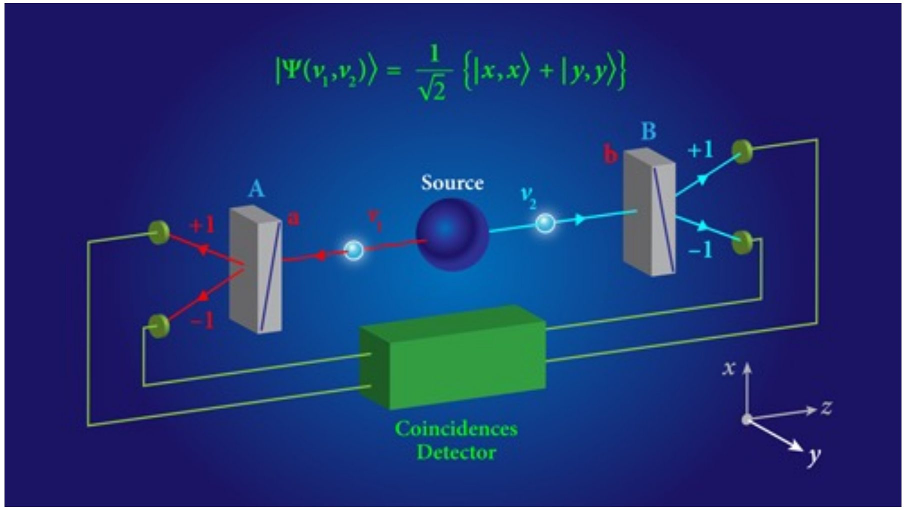
^{1}H																	^{2}He
^{3}Li	^{4}Be											^{5}B	^{6}C	^{7}N	^{8}O	^{9}F	^{10}Ne
^{11}Na	^{12}Mg											^{13}Al	^{14}Si	^{15}P	^{16}S	^{17}Cl	^{18}Ar
^{19}K	^{20}Ca	^{21}Sc	^{22}Ti	^{23}V	^{24}Cr	^{25}Mn	^{26}Fe	^{27}Co	^{28}Ni	^{29}Cu	^{30}Zn	^{31}Ga	^{32}Ge	^{33}As	^{34}Se	^{35}Br	^{36}Kr
^{37}Rb	^{38}Sr	^{39}Y	^{40}Zr	^{41}Nb	^{42}Mo	^{43}Tc	^{44}Ru	^{45}Rh	^{46}Pd	^{47}Ag	^{48}Cd	^{49}In	^{50}Sn	^{51}Sb	^{52}Te	^{53}I	^{54}Xe
^{55}Cs	^{56}Ba	*	^{72}Hf	^{73}Ta	^{74}W	^{75}Re	^{76}Os	^{77}Ir	^{78}Pt	^{79}Au	^{80}Hg	^{81}Tl	^{82}Pb	^{83}Bi	^{84}Po	^{85}At	^{86}Rn
^{87}Fr	^{88}Ra	+															
* Lanthanides			^{57}La	^{58}Ce	^{59}Pr	^{60}Nd	^{61}Pm	^{62}Sm	^{63}Eu	^{64}Gd	^{65}Tb	^{66}Dy	^{67}Ho	^{68}Er	^{69}Tm	^{70}Yb	^{71}Lu
+ Actinides			^{89}Ac	^{90}Th	^{91}Pa	^{92}U	^{93}Np	^{94}Pu	^{95}Am	^{96}Cm	^{97}Bk	^{98}Cf	^{99}Es				

$\ell = 3$

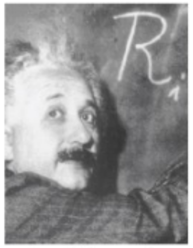
http://physics.nist.gov/PhysRefData/Handbook/periodictable.htm

Section 10

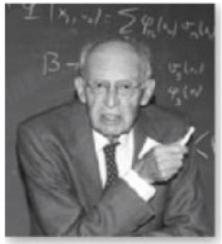
EPR paradox and Bell inequality

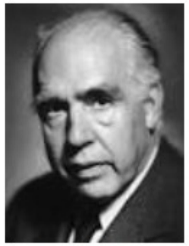


The EPR argument


A. Einstein


B. Podolsky


N. Rosen


N. Bohr

MAY 15, 1935 PHYSICAL REVIEW VOLUME 47

Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?

A. EINSTEIN, B. PODOLSKY AND N. ROSEN, *Institute for Advanced Study, Princeton, New Jersey*

(Received March 25, 1935)

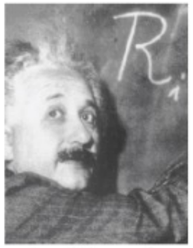
In 1935, EPR said the quantum theory is not complete pointing out the existence of possible hidden variables in the formalism

Einstein discovered that the formalism of quantum mechanics contains the existence of particular states named entangled states

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|{+}{+}\rangle + |{-}{-}\rangle\right]$$

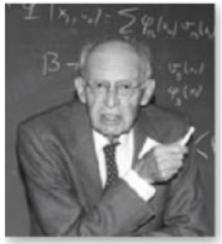
"If, without in any way disturbing a system, we can predict with certainty the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity"

The EPR argument

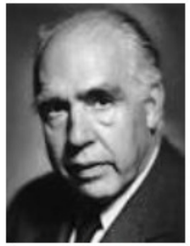


A. Einstein

B. Podolsky



N. Rosen



N. Bohr

MAY 15, 1935 PHYSICAL REVIEW VOLUME 47

Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?

A. EINSTEIN, B. PODOLSKY AND N. ROSEN, *Institute for Advanced Study, Princeton, New Jersey*

(Received March 25, 1935)

In 1935, Niels Bohr answered EPR by saying that the quantum theory is complete i.e. there are no hidden variables

OCTOBER 15, 1935 PHYSICAL REVIEW VOLUME 48

Can Quantum-Mechanical Description of Physical Reality be Considered Complete?

N. BOHR, *Institute for Theoretical Physics, University, Copenhagen*

(Received July 13, 1935)

In 1964, John Bells introduced an inequality that has further led to the experimental evidence that quantum mechanics is indeed complete

Entangled state

An entangled system is defined to be one whose quantum state cannot be factored as a product of states of its local constituents; that is to say, they are not individual particles but are an inseparable whole

Let us consider two vectors $|\psi_1\rangle = \sum_n a_n|\phi_n^{(1)}\rangle$ et $|\psi_2\rangle = \sum_p b_p|\phi_p^{(2)}\rangle$ then

$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle = \sum_{n,p} a_n\, b_p\, |\phi_n^{(1)}\rangle \otimes |\phi_p^{(2)}\rangle$ is a vector of the total Hilbert space $\mathcal{H}_1^M \otimes \mathcal{H}_2^N$

However the reverse statement is wrong i.e. there exists non separable states of the Hilbert Space that can not be expressed as

$$|\psi\rangle = \sum_{n,p} c_{n,p}\, |\phi_n^{(1)}\rangle \otimes |\phi_p^{(2)}\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle = \sum_{n,p} a_n\, b_p\, |\phi_n^{(1)}\rangle \otimes |\phi_p^{(2)}\rangle$$

Such a general state Ψ which cannot be written in the form of a tensor product is called an entangled state

Quiz 12

An entangled system is defined to be one whose quantum state cannot be factored as a product of states of its local constituents.
A non separable state is entangled

Find below which of the following quantum states are entangled?

$$|++\rangle = |a:+\rangle \otimes |b:+\rangle$$

A. $|++\rangle$

B. $|+-\rangle$

C. $(|++\rangle + |+-\rangle)/\sqrt{2}$

D. $(|++\rangle + |--\rangle)/\sqrt{2}$

E. $(|+-\rangle + |-+\rangle)/\sqrt{2}$

F. $(|++\rangle + |+-\rangle + |-+\rangle + |--\rangle)/2$

Quiz 12

An entangled system is defined to be one whose quantum state cannot be factored as a product of states of its local constituents.

A non separable state is entangled

Find below which of the following quantum states are entangled?

$$|++\rangle = |a:+\rangle \otimes |b:+\rangle$$

A. $|++\rangle$

B. $|+-\rangle$

C. $(|++\rangle + |+-\rangle)/\sqrt{2}$ $\rightarrow$ $|+\rangle \otimes \left(\dfrac{|+\rangle + |-\rangle}{\sqrt{2}}\right)$

D. $(|++\rangle + |--\rangle)/\sqrt{2}$

E. $(|+-\rangle + |-+\rangle)/\sqrt{2}$

F. $(|++\rangle + |+-\rangle + |-+\rangle + |--\rangle)/2$ $\rightarrow$ $\dfrac{(|+\rangle + |-\rangle) \otimes (|+\rangle + |-\rangle)}{2}$

Photon polarization

The polarization of a single photon is described in an Hilbert space of dimension 2

$$|\psi\rangle = \alpha\,|\mathrm{v}\rangle + \beta\,|\mathrm{h}\rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$

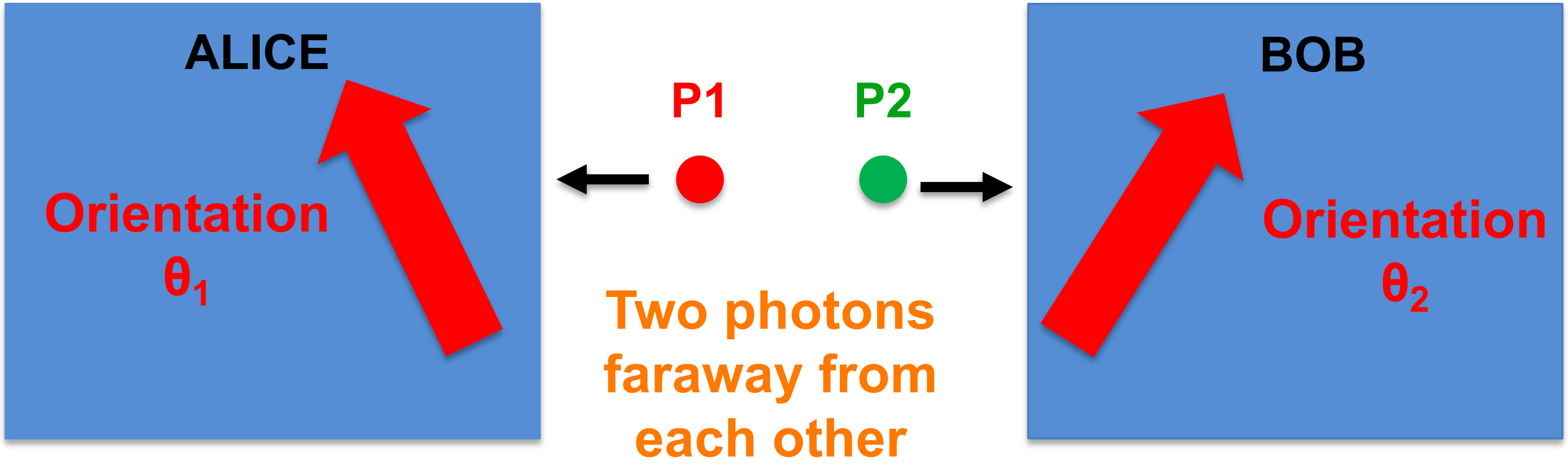
(α, β) real coefficients: linear polarizations
(α, β) complex coefficients: elliptic and circular polarizations

An individual photon can be described as having right or left circular polarization, or a superposition of the two. Equivalently, a photon can be described as having horizontal or vertical linear polarization, or a superposition of the two

→ It is a two-state quantum system called quantum bit or qbit

Applications: quantum cryptography & quantum information

Measurement on an entangled state



Consider the following entangled quantum configuration with two photons linearly polarized

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|P1:h_1\rangle \otimes |P2:h_2\rangle + |P1:v_1\rangle \otimes |P2:v_2\rangle\right]$$

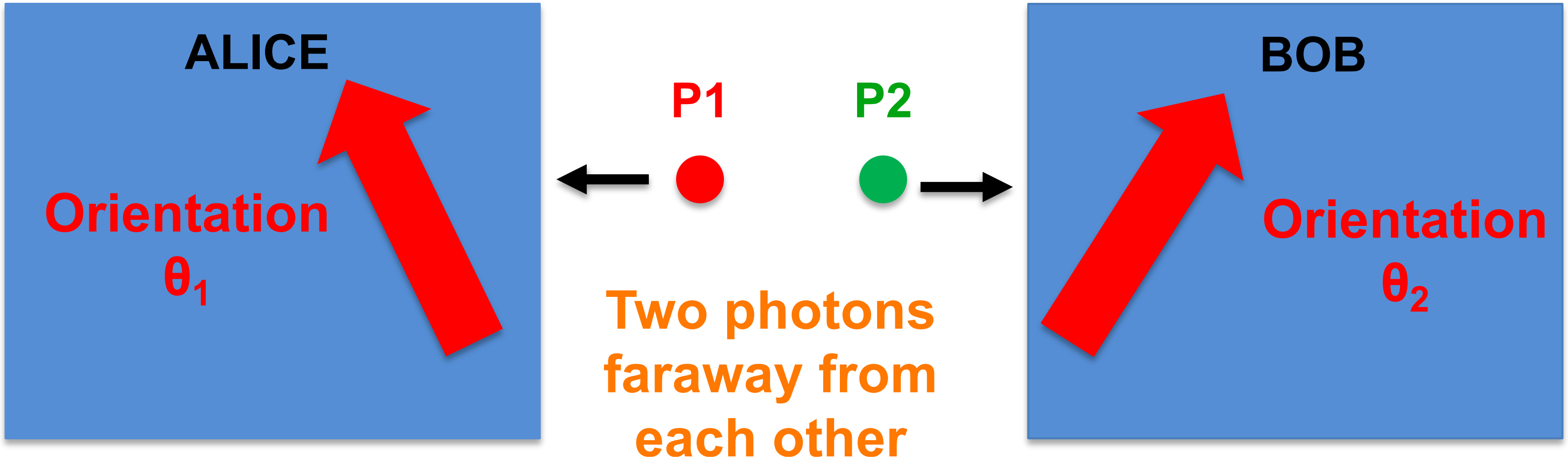
$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|h_1 h_2\rangle + |v_1 v_2\rangle\right] \Longleftrightarrow |\Psi\rangle = \frac{1}{\sqrt{2}}\left[|{+}{+}\rangle + |{-}{-}\rangle\right]$$

$$\mathcal{E} = \mathcal{E}_{P_1} \otimes \mathcal{E}_{P_2}$$

The Hilbert space of dimension 4

$$\dim \mathcal{E} = \dim \mathcal{E}_{P_1} \times \dim \mathcal{E}_{P_2}$$

Measurement on an entangled state



$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|h_1 h_2\rangle + |v_1 v_2\rangle\right]$$

P1 transmitted
Result (eigenvalue): ε_1=+1
Eigenstates: $|+_{\theta 1}\rangle$

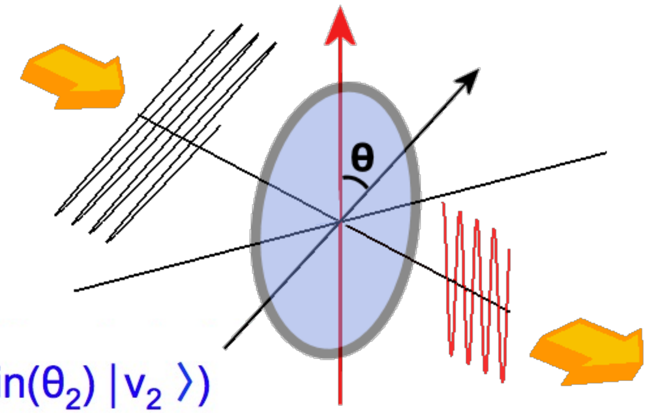
P2 transmitted
Result (eigenvalue): ε_2=+1
Eigenstates: $|+_{\theta 2}\rangle$

P1 reflected
Result (eigenvalue): ε_1=-1
Eigenstates: $|-_{\theta 1}\rangle$

P2 reflected
Result (eigenvalue): ε_1=-1
Eigenstates: $|-_{\theta 2}\rangle$

Measurement on an entangled state

Initial entangled quantum state



$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|h_1 h_2\rangle + |v_1 v_2\rangle\right]$$

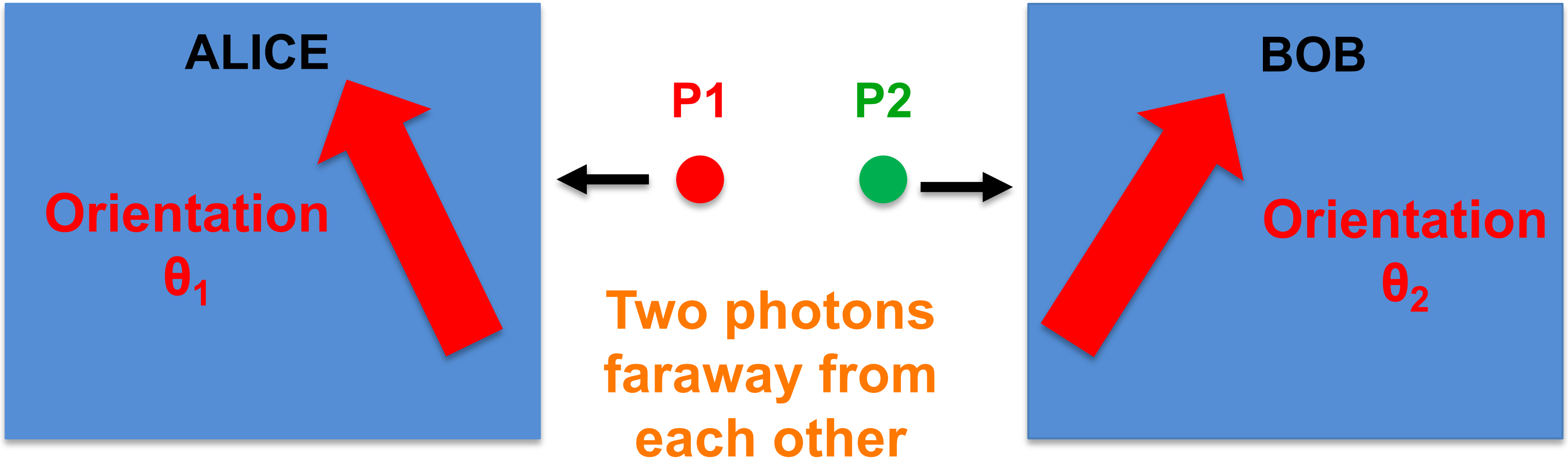
$$\begin{aligned}
|+_{\theta1}, +_{\theta2}\rangle &= (\cos(\theta_1)|h_1\rangle + \sin(\theta_1)|v_1\rangle) \otimes (\cos(\theta_2)|h_2\rangle + \sin(\theta_2)|v_2\rangle) \\
&= \cos(\theta_1)\cos(\theta_2)\,|h_1 h_2\rangle + \sin(\theta_1)\cos(\theta_2)\,|v_1 h_2\rangle + \\
&\qquad \cos(\theta_1)\sin(\theta_2)\,|h_1 v_2\rangle + \sin(\theta_1)\sin(\theta_2)\,|v_1 v_2\rangle
\end{aligned}$$

$$\begin{aligned}
|+_{\theta1}, -_{\theta2}\rangle &= (\cos(\theta_1)|h_1\rangle + \sin(\theta_1)|v_1\rangle) \otimes (-\sin(\theta_2)|h_2\rangle + \cos(\theta_2)|v_2\rangle) \\
&= -\cos(\theta_1)\sin(\theta_2)\,|h_1 h_2\rangle - \sin(\theta_1)\sin(\theta_2)\,|v_1 h_2\rangle + \\
&\qquad \cos(\theta_1)\cos(\theta_2)\,|h_1 v_2\rangle + \sin(\theta_1)\cos(\theta_2)\,|v_1 v_2\rangle
\end{aligned}$$

$$\begin{aligned}
|-_{\theta1}, +_{\theta2}\rangle &= (-\sin(\theta_1)|h_1\rangle + \cos(\theta_1)|v_1\rangle) \otimes (\cos(\theta_2)|h_2\rangle + \sin(\theta_2)|v_2\rangle) \\
&= -\sin(\theta_1)\cos(\theta_2)\,|h_1 h_2\rangle + \cos(\theta_1)\cos(\theta_2)\,|v_1 h_2\rangle - \\
&\qquad \sin(\theta_1)\sin(\theta_2)\,|h_1 v_2\rangle + \cos(\theta_1)\sin(\theta_2)\,|v_1 v_2\rangle
\end{aligned}$$

$$\begin{aligned}
|-_{\theta1}, -_{\theta2}\rangle &= (-\sin(\theta_1)|h_1\rangle + \cos(\theta_1)|v_1\rangle) \otimes (-\sin(\theta_2)|h_2\rangle + \cos(\theta_2)|v_2\rangle) \\
&= \sin(\theta_1)\sin(\theta_2)\,|h_1 h_2\rangle - \cos(\theta_1)\sin(\theta_2)\,|v_1 h_2\rangle - \\
&\qquad \sin(\theta_1)\cos(\theta_2)\,|h_1 v_2\rangle + \cos(\theta_1)\cos(\theta_2)\,|v_1 v_2\rangle
\end{aligned}$$

Measurement on an entangled state



$$|+_{\theta 1}, +_{\theta 2}\rangle = (\cos(\theta_1)\,|h_1\rangle + \sin(\theta_1)\,|v_1\rangle) \otimes (\cos(\theta_2)\,|h_2\rangle + \sin(\theta_2)\,|v_2\rangle)$$

$$P(+_{\theta 1}, +_{\theta 2}) = |\langle +_{\theta 1}, +_{\theta 2}|\Psi\rangle|^2 = \tfrac{1}{2}\cos^2(\theta_2 - \theta_1)$$

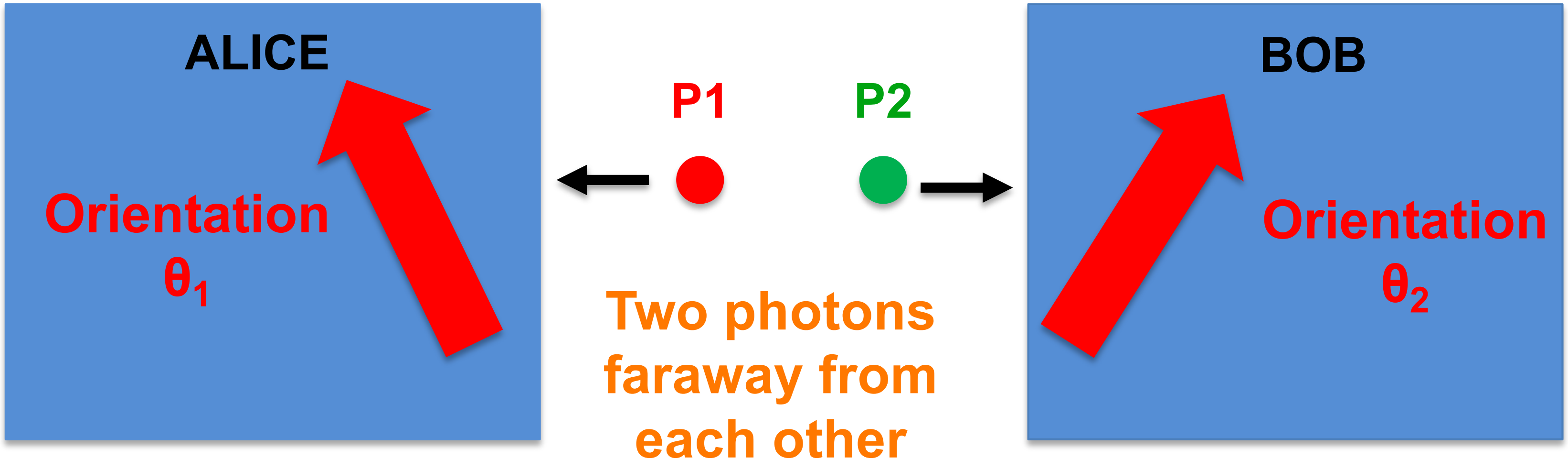
$$P(-_{\theta 1}, -_{\theta 2}) = |\langle -_{\theta 1}, -_{\theta 2}|\Psi\rangle|^2 = \tfrac{1}{2}\cos^2(\theta_2 - \theta_1)$$

$$P(+_{\theta 1}, -_{\theta 2}) = |\langle +_{\theta 1}, -_{\theta 2}|\Psi\rangle|^2 = \tfrac{1}{2}\sin^2(\theta_2 - \theta_1)$$

$$P(-_{\theta 1}, +_{\theta 2}) = |\langle -_{\theta 1}, +_{\theta 2}|\Psi\rangle|^2 = \tfrac{1}{2}\sin^2(\theta_2 - \theta_1)$$

The sum of the joint probabilities is 1

Measurement on an entangled state



$$P(+_{\theta1}, +_{\theta2}) = |\langle +_{\theta1}, +_{\theta2} | \Psi \rangle|^2 = \tfrac{1}{2}\cos^2(\theta_2 - \theta_1)$$

$$P(-_{\theta1}, -_{\theta2}) = |\langle -_{\theta1}, -_{\theta2} | \Psi \rangle|^2 = \tfrac{1}{2}\cos^2(\theta_2 - \theta_1)$$

$$P(+_{\theta1}, -_{\theta2}) = |\langle +_{\theta1}, -_{\theta2} | \Psi \rangle|^2 = \tfrac{1}{2}\sin^2(\theta_2 - \theta_1)$$

$$P(-_{\theta1}, +_{\theta2}) = |\langle -_{\theta1}, +_{\theta2} | \Psi \rangle|^2 = \tfrac{1}{2}\sin^2(\theta_2 - \theta_1)$$

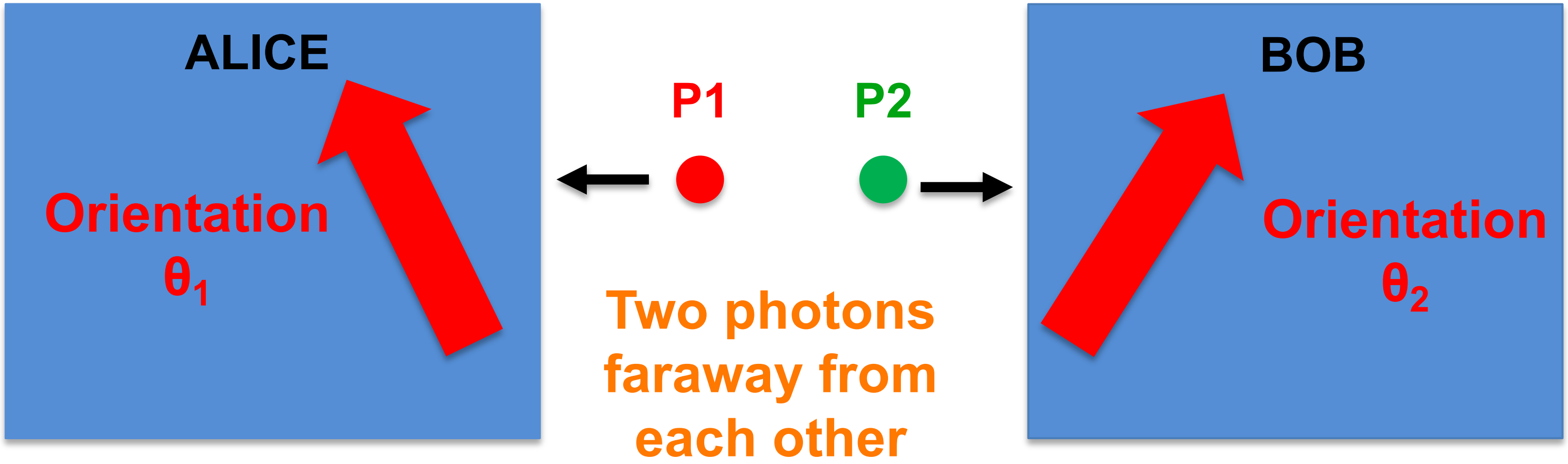
What are the single probabilities for separated results?

$$P(+_{\theta1}) = P(+_{\theta1}, +_{\theta2}) + P(+_{\theta1}, -_{\theta2}) = \tfrac{1}{2}$$

$$P(-_{\theta1}) = P(+_{\theta2}) = P(-_{\theta2}) = \tfrac{1}{2}$$

Randomness results not dependent on the polarizer angles. However those obtained by Alice and Bob together are strongly correlated

Measurement on an entangled state



For each pair of particles, Alice and Bob calculate the product of the results $\varepsilon_1 = \pm 1$ and $\varepsilon_2 = \pm 1$ and obtained a number $\varepsilon_1\varepsilon_2 = \pm 1$

→ $\varepsilon_1\varepsilon_2 = +1$ results are correlated; $\varepsilon_1\varepsilon_2 = -1$ results are not correlated

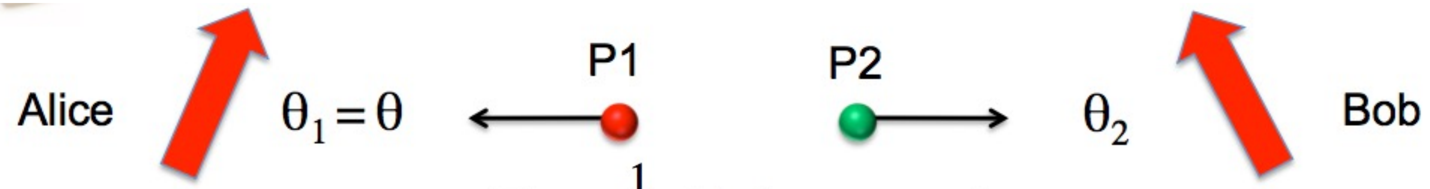
Repeating the measurements multiple times, Alice and Bob can obtain the correlation function

$$E(\theta_1, \theta_2) = \langle \epsilon_1 \epsilon_2 \rangle \qquad | E(\theta_1, \theta_2) | \leq 1$$

$$E(\theta_1, \theta_2) = \sum_k (\epsilon_1 \epsilon_2)_k P_k(\epsilon_1, \epsilon_2) = \cos^2(\theta_2 - \theta_1) - \sin^2(\theta_2 - \theta_1) = \cos[2(\theta_2 - \theta_1)]$$

Quiz 13

Correlation on an entangled states?



$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|h_1 h_2\rangle + |v_1 v_2\rangle\right]$$

A. $E(\theta, \theta) = +1$

B. $E(\theta, \theta) = 0$

C. $E(\theta, \theta + 45°) = 0$

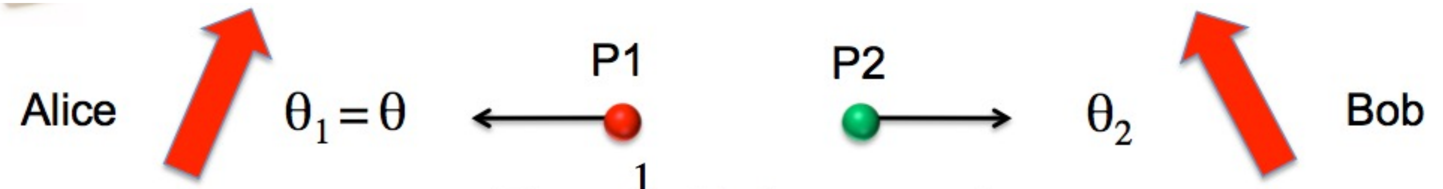
D. $E(\theta, \theta + 45°) = -1$

E. $E(\theta, \theta + 90°) = 0$

F. $E(\theta, \theta + 90°) = -1$

Quiz 13

Correlation on an entangled states



$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|h_1 h_2\rangle + |v_1 v_2\rangle\right]$$

A. $E(\theta, \theta) = +1$

B. $E(\theta, \theta) = 0$

C. $E(\theta, \theta + 45°) = 0$

D. $E(\theta, \theta + 45°) = -1$

E. $E(\theta, \theta + 90°) = 0$

F. $E(\theta, \theta + 90°) = -1$

When $\theta_1=\theta_2$ Alice and Bob will always find the same results (++) or (--)

When $\theta_2=\theta_1+90°$ Alice and Bob will always find opposite results (+-) or (-+)

Measurement on an entangled state

Now consider the case for which $\theta_1=\theta$ Alice has measured +1
What is the state of the system after her measurement but before Bob's measurement?

Third postulate: The quantum state is obtained by projection. However if Bob has not yet performed the measurement, we replace the corresponding projector by the identity

Proof (not trivial)

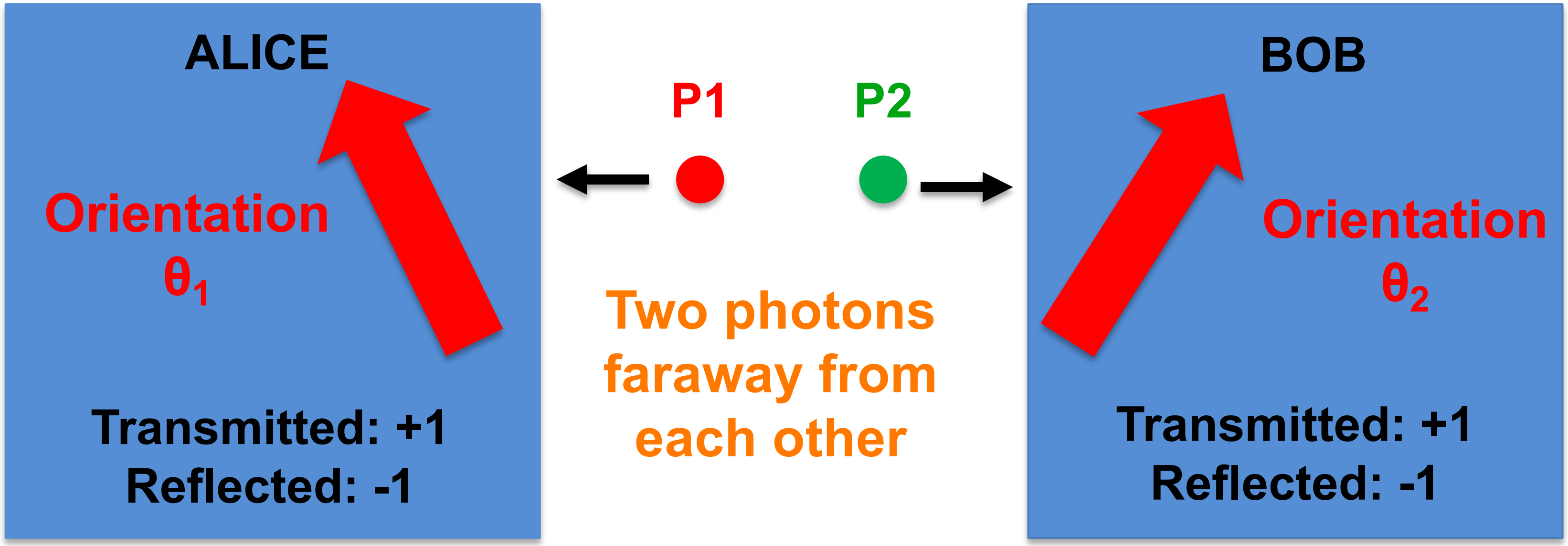
$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[\left|+_\theta, +_{\theta_2}\right\rangle + \left|-_\theta, -_{\theta_2}\right\rangle\right]$$

$$\left|\Psi_p\right\rangle = \left(\left|+_\theta\right\rangle\left\langle+_\theta\right| \otimes \mathbb{1}_2\right)|\Psi\rangle = \frac{1}{\sqrt{2}}\left|+_\theta, +_{\theta_2=\theta}\right\rangle$$

If Alice measure $\left|+_{\theta_1=\theta}\right\rangle$, the state received by Bob is $\left|+_{\theta_2=\theta}\right\rangle$

Now, you should start wondering about metaphysical questions…

Bell inequality



How to explain quantum correlations? Following the EPR argument, John Bell assumed that there exists hidden parameters λ that must determine the outcome of Alice and Bob measurements

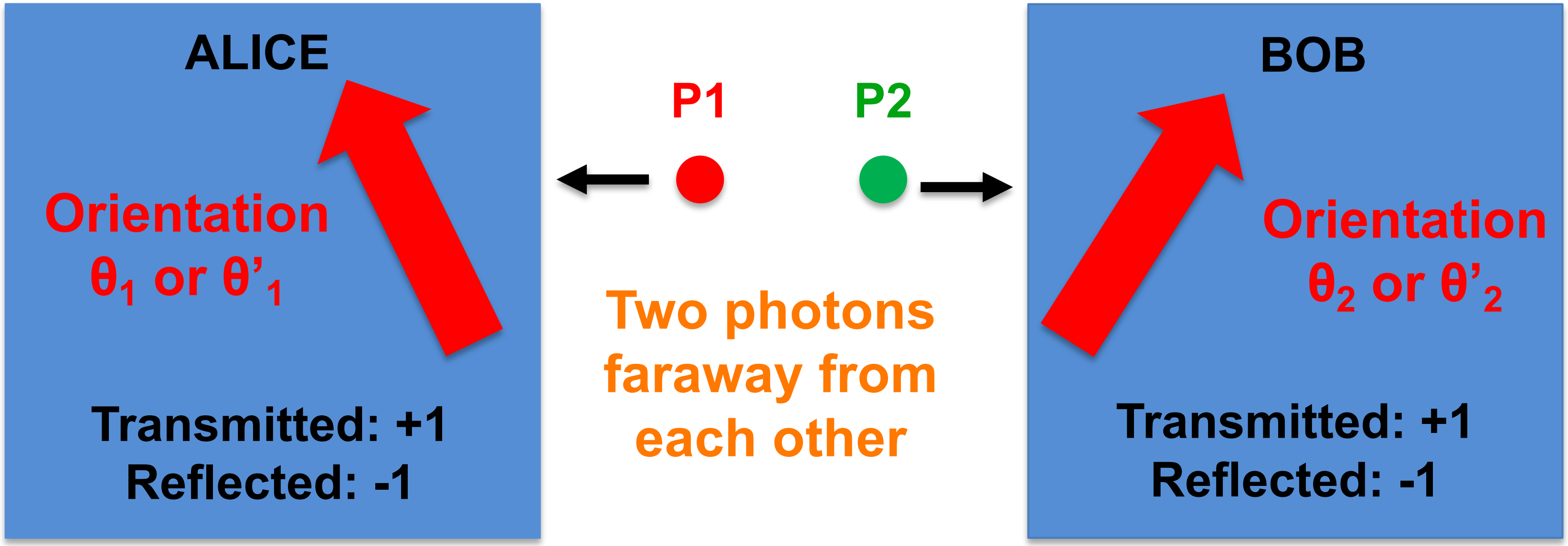
$$A(\theta_1, \lambda) = \pm 1$$

$$B(\theta_2, \lambda) = \pm 1$$

$$E(\theta_1, \theta_2) = \int A(\theta_1, \lambda) B(\theta_2, \lambda) \overbrace{\rho(\lambda)}^{\text{Statistic distribution (normalized)}} d\lambda$$

J.S. Bell, Rev. Mod. Phys. 38, 447 (1966)

Bell inequality



Then John Bell introduced the following quantity (averaging on $\rho(\lambda)$)

$$S = E(\theta_1, \theta_2) + E(\theta'_1, \theta_2) + E(\theta'_1, \theta'_2) - E(\theta_1, \theta'_2)$$

$$s = \langle S \rangle = A(\theta_1, \lambda)B(\theta_2, \lambda) + A(\theta'_1, \lambda)B(\theta_2, \lambda) + A(\theta'_1, \lambda)B(\theta'_2, \lambda) - A(\theta_1, \lambda)B(\theta'_2, \lambda) = \pm 2$$

For any hidden variable theory, Bell inequality tells us

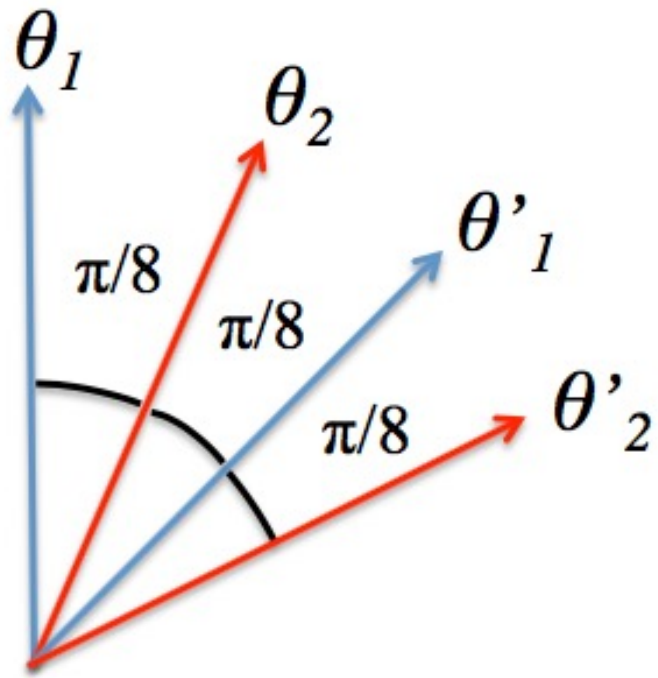
$$| S | \leq 2$$

J.S. Bell, Rev. Mod. Phys. 38, 447 (1966)

Violation of Bell inequality

Entangled state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left[|h_1 h_2\rangle + |v_1 v_2\rangle\right]$$



From quantum mechanics, we know the correlation function

$$E(\theta_1, \theta_2) = \cos[2(\theta_2 - \theta_1)]$$

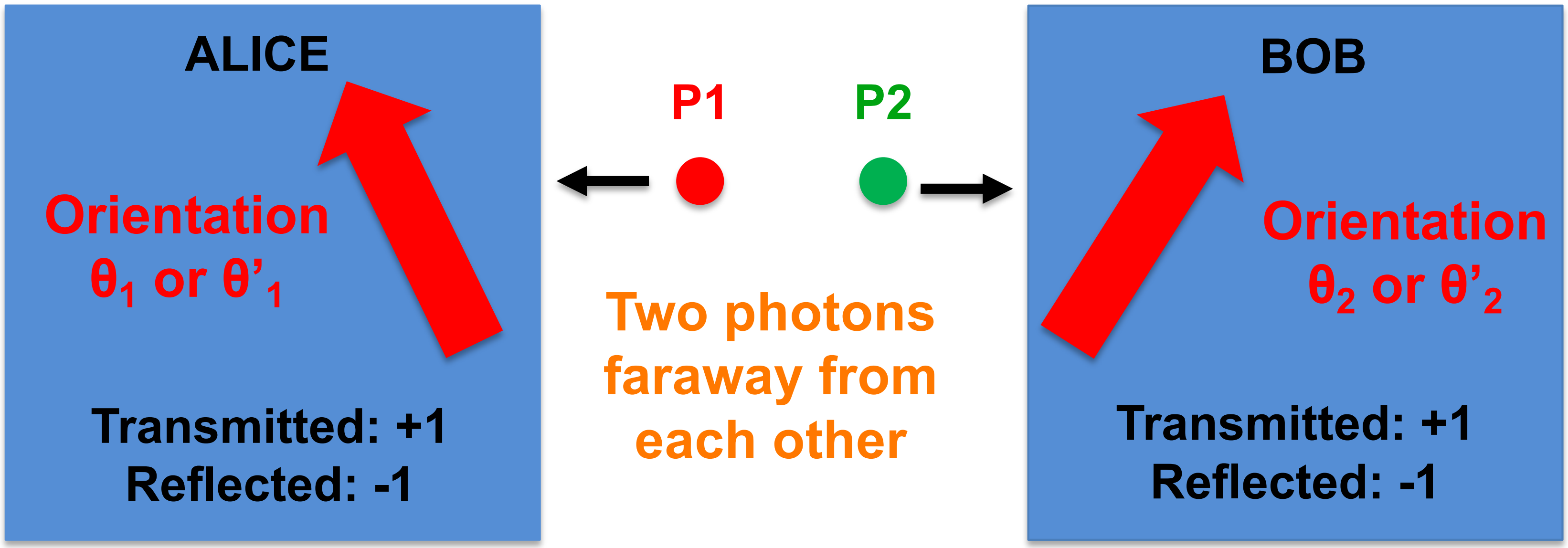
$$S = E(\theta_1, \theta_2) + E(\theta'_1, \theta_2) + E(\theta'_1, \theta'_2) - E(\theta_1, \theta'_2)$$

$$S = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} - \frac{-1}{\sqrt{2}}$$

$$|S| = 2\sqrt{2} > 2$$

Violation of Bell inequality!!

Bell inequality



How can we explain this result with such "simple assumptions"?

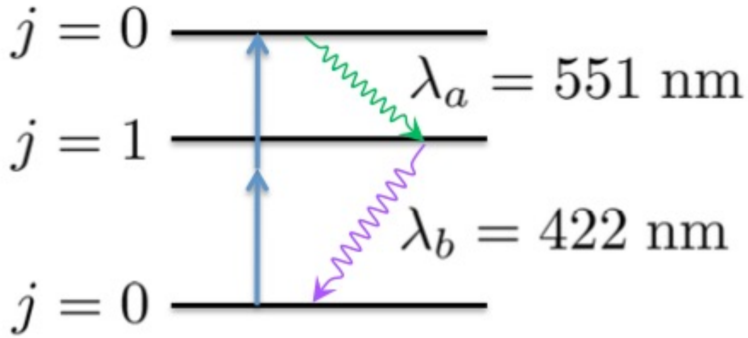
$$A(\theta_1\,,\lambda) = \pm\,1 \qquad B(\theta_2\,,\lambda) = \pm\,1 \qquad \int \rho(\lambda)d\lambda = 1$$

Bell assumptions are always verified in classical physics but there is no weakness behind them

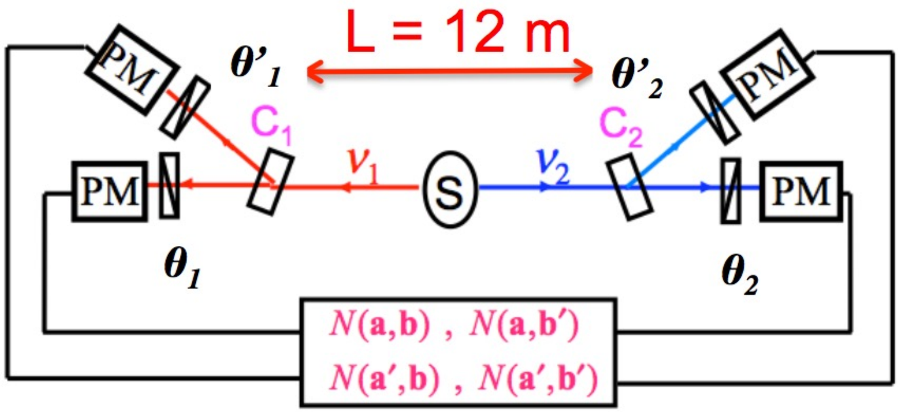
1. **Local model** $A(\theta_1\,,\cancel{\theta_2}\,,\lambda) = \pm\,1 \qquad B(\cancel{\theta_1}\,,\theta_2\,,\lambda) = \pm\,1$

2. **The hidden properties are hold by the each particles via the variable λ (Bohr: "This statement is not true in quantum mechanics")**

Aspect experiments (1981-82)



C_1, C_2 are optical switches redirecting photons towards polarizers with angles (θ_1,θ'_1) and (θ_2,θ'_2). Commutation was faster (10 ns) than propagation of light between polarizers (40 ns) and even faster than time of flight of photons between the source and each switch (20 ns)



A. Aspect, P. Grangier, G. Roger, Phys. Rev. Lett. 49, 91 (1982)
A. Aspect, J. Dalibard, G. Roger, Phys. Rev. Lett. 49, 1804 (1982)

Aspect experiments (1981-82)

Result in a perfect agreement with quantum theory

$$E(\theta_1,\theta_2) = \cos[2(\theta_2 - \theta_1)]$$

$$S = E(\theta_1,\theta_2) + E(\theta_1',\theta_2) + E(\theta_1',\theta_2') - E(\theta_1,\theta_2')$$

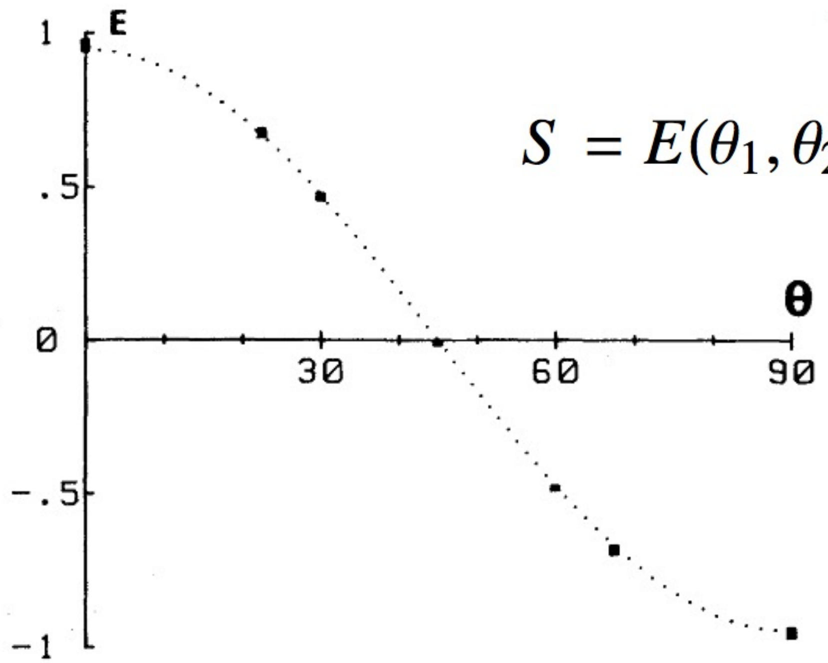


FIG. 3. Correlation of polarizations as a function of the relative angle of the polarimeters. The indicated errors are ±2 standard deviations. The dotted curve is not a fit to the data, but quantum mechanical predictions for the actual experiment. For ideal polarizers, the curve would reach the values ±1.

$S_{exp} = 2.697 \pm 0.015$

Others experiments

Aspect experiments were pioneered and showed (fairly) conclusively that quantum physics is non-local, and that the universe is much stranger than it appears, or than Einstein would've liked it to be

Others ultimate experiments have been done in 2015
Entangled photon pair, L = 58 m in Vienna, Austria Vienne [1]
Entangled photon pair, L = 185 m in Boulder, USA [2]
Entangled spin pair, L = 1.3 km in Delft, The Netherlands [3]

→ All results are in a perfect agreement with quantum theory
→ Closing the door on Einstein and Bohr's quantum debate!

[1] M. Giustina et al., Phys. Rev. Lett. 115, 250401 (2015)
[2] L. K. Shalm et al., Phys. Rev. Lett. 115, 250402 (2015)
[3] B. Hensen et al., Nature 526, 682 (2015)

See also, https://physics.aps.org/articles/v8/123

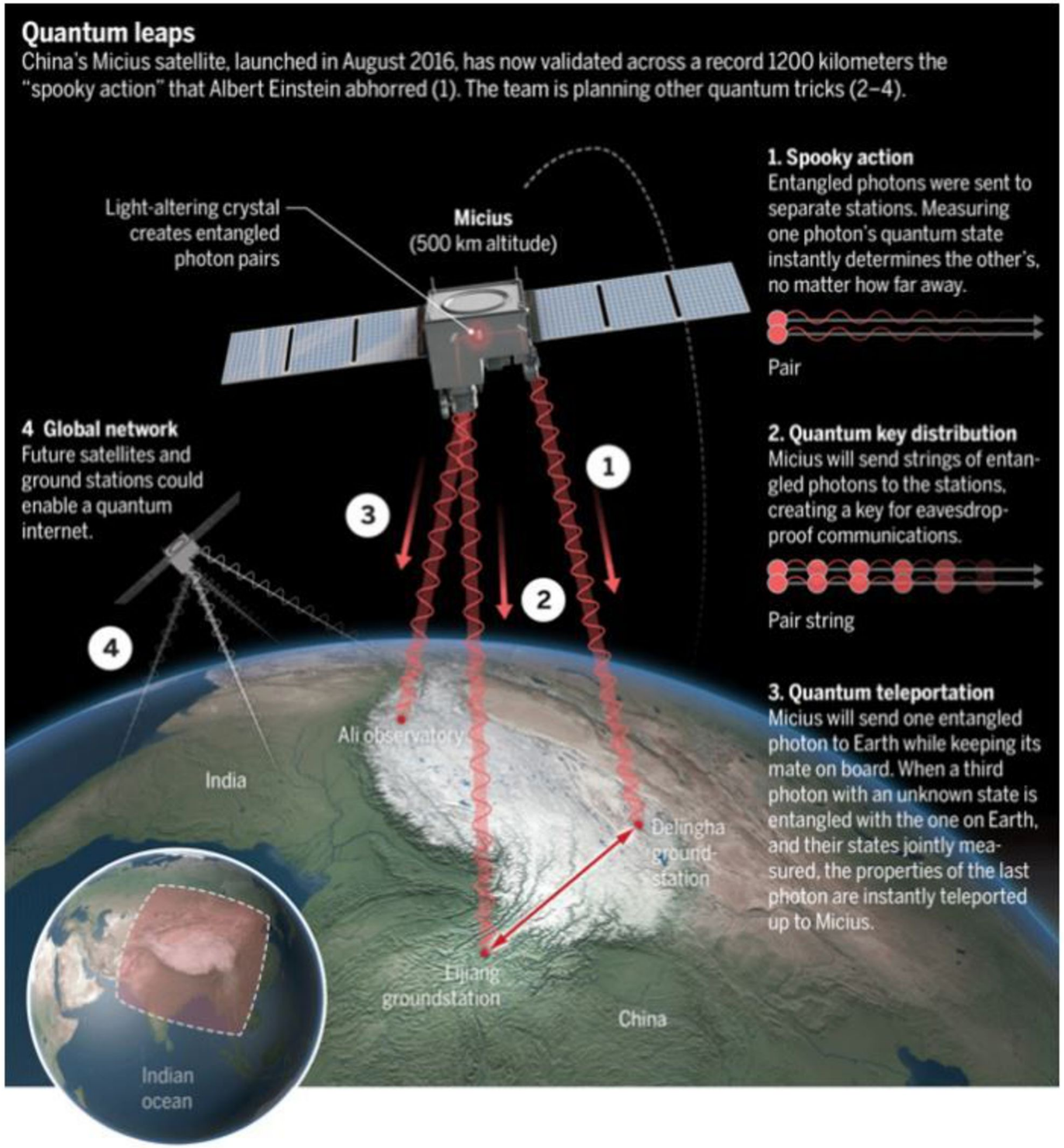
Consequences of the violation of Bell inequality

This conclusively shows that either the realism and/or locality assumptions must be voided, i.e., there is no deeper local realist theory lurking behind quantum mechanics. Most physicists have chosen to reject realism (i.e., that unobserved quantities have definite values), though some still favor nonlocal realist theories

In any case, entanglement allows us to introduce and manipulate nonlocal correlations, a concept alien to most conventional classical physics. It is this property that enables many of the novel uses of quantum information

Multiple applications: quantum cryptography, quantum key-distribution (QKD), quantum teleportation, quantum computation ,
See supplementary information IV for further readings

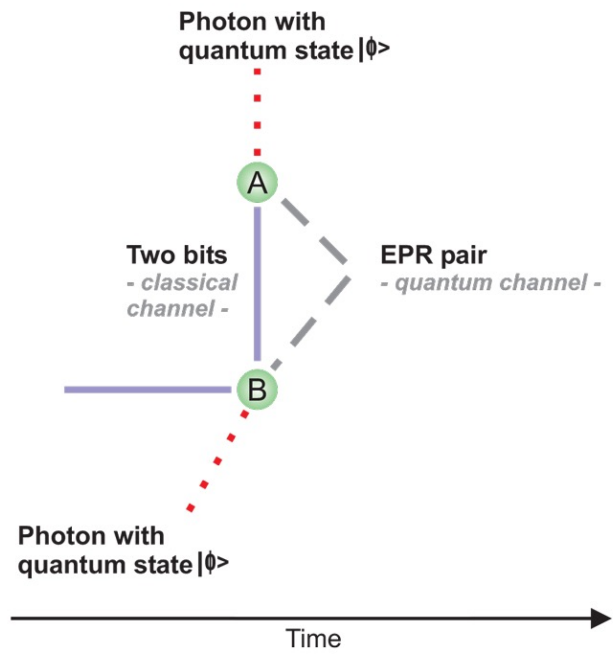
Quantum teleportation



RESEARCH ARTICLE

QUANTUM OPTICS

Satellite-based entanglement distribution over 1200 kilometers



Science, Vol. 356, 6343, pp. 1140-1144, 2017

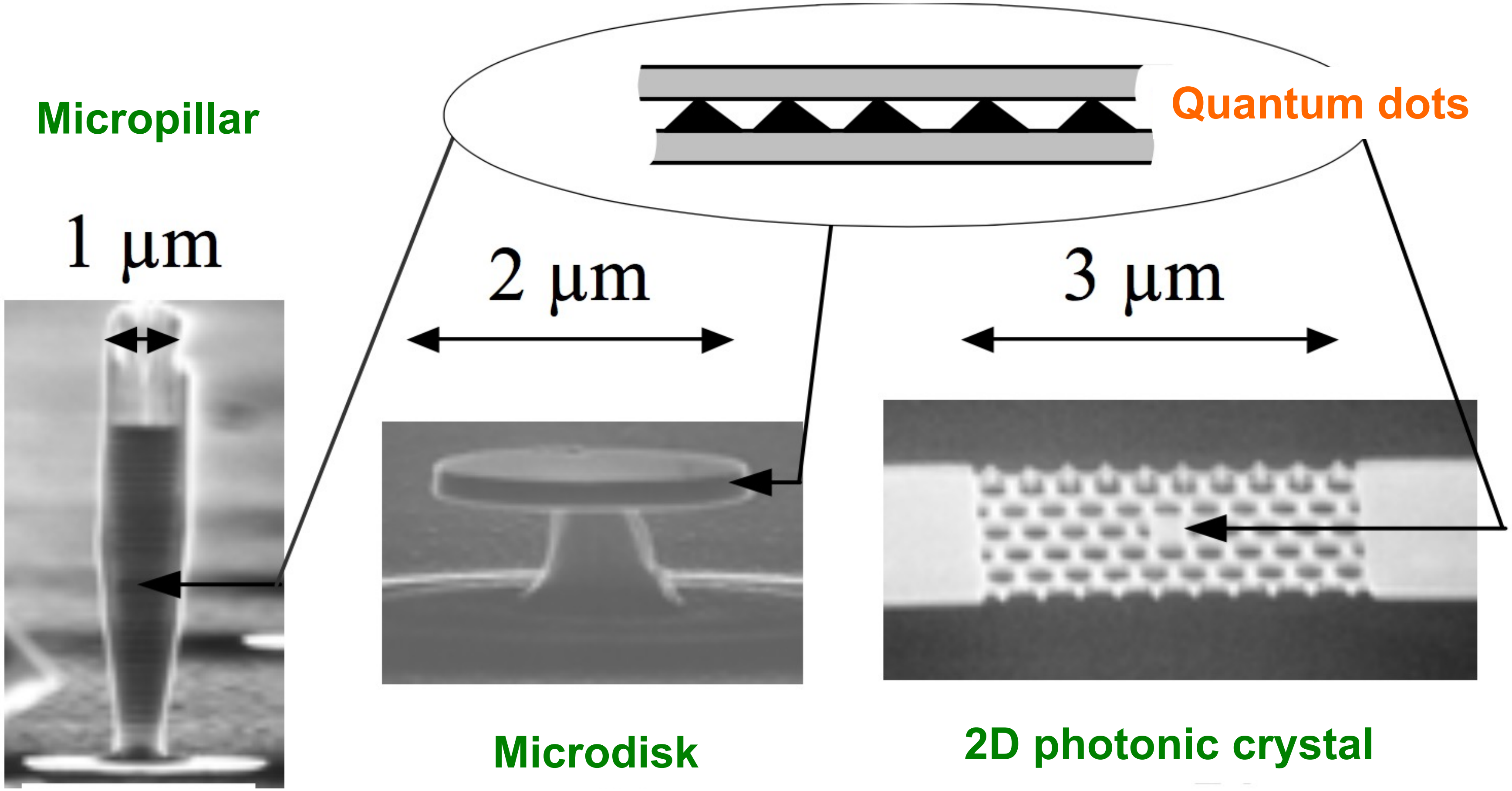
Section 12

Quantization of Electromagnetic Field

$$\hat{H}_{\vec{k},\lambda} = \frac{\epsilon_0 \mathcal{V}}{2}\hat{e}^2_{\vec{k},\lambda} + \frac{\mu_0 \mathcal{V}}{2}\hat{h}^2_{\vec{k},\lambda}$$

It is recommended to also read the supplementary information V

Multiple applications at the nanoscales



The quantization of the field is required to understand the light-matter interaction at the nanoscale

Maxwell equations

In free-space, recall Maxwell equations (with J=0 and ρ=0)

$$\vec{\nabla} \cdot (\epsilon_0 \vec{E}) = 0 \qquad \vec{\nabla} \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t}$$

$$\vec{\nabla} \cdot (\mu_0 \vec{H}) = 0 \qquad \mu_0^{-1} \vec{\nabla} \times \vec{H} = \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

These equations describe classical electromagnetic waves.
But how do we get to a quantum theory of electromagnetic radiation?
→ We can find the classical Hamiltonian for electromagnetic waves and quantize it

Consider a perfect cubic cavity of volume $\mathcal{V} = L^3$ as $L \rightarrow +\infty$
We want to find the electromagnetic modes in the box and quantize them

Electromagnetic modes & spatial profiles

Modes are written in terms of the fields (using separation of variables)

$$\vec{E}_{\vec{k},\lambda}(\vec{r},t) = \vec{u}_{\vec{k},\lambda}(\vec{r})e_{\vec{k},\lambda}(t) \quad \text{and} \quad \vec{H}_{\vec{k},\lambda}(\vec{r},t)_{\vec{k},\lambda} = \vec{v}_{\vec{k},\lambda}(\vec{r})h_{\vec{k},\lambda}(t)$$

with

$$\vec{u}_{\vec{k},\lambda} = \vec{C}_1 \sin(\vec{k}\cdot\vec{r})$$

$$\vec{v}_{\vec{k},\lambda} = \vec{C}_2 \cos(\vec{k}\cdot\vec{r})$$

Normalization conditions

$$\int_{\mathcal{V}} |\vec{u}_{\vec{k},\lambda}(\vec{r})|^2 d\vec{r} = \mathcal{V} \qquad \int_{\mathcal{V}} |\vec{v}_{\vec{k},\lambda}(\vec{r})|^2 d\vec{r} = \mathcal{V}$$

Energy per mode

$$\mathcal{E}_{\vec{k},\lambda} = \frac{1}{2}\int_{\mathcal{V}} d\vec{r}\left[\epsilon_0 \vec{E}^2_{\vec{k},\lambda}(\vec{r}) + \mu_0 \vec{H}^2_{\vec{k},\lambda}(\vec{r})\right]$$

Electromagnetic modes & spatial profiles

Plugging the fields into Maxwell's equations

$$\frac{\partial e_{\vec{k},\lambda}(t)}{\partial t} = \frac{k}{\epsilon_0} h_{\vec{k},\lambda}(t) \qquad \frac{\partial h_{\vec{k},\lambda}(t)}{\partial t} = -\frac{k}{\mu_0} e_{\vec{k},\lambda}(t)$$

The solutions for this set of equations are oscillatory with frequency

$\omega_k = \frac{k}{\sqrt{\epsilon_0 \mu_0}} = ck$ **and $\vec{h}$ and $\vec{e}$ will be 90°out of phase**

Energy per mode becomes

$$\begin{aligned}
\mathcal{E}_{\vec{k},\lambda} &= \frac{1}{2} \int_{\mathcal{V}} d\vec{r} \left(\epsilon_0 \vec{E}^2_{\vec{k},\lambda}(\vec{r},t) + \mu_0 \vec{H}^2_{\vec{k},\lambda}(\vec{r},t) \right) \\
&= \frac{1}{2} \epsilon_0 e^2_{\vec{k},\lambda}(t) \int_{\mathcal{V}} |\vec{u}_{\vec{k},\lambda}|^2 d\vec{r} + \frac{1}{2} \mu_0 h^2_{\vec{k},\lambda}(t) \int_{\mathcal{V}} |\vec{v}_{\vec{k},\lambda}|^2 d\vec{r} \\
&= \frac{\epsilon_0 \mathcal{V}}{2} e^2_{\vec{k},\lambda}(t) + \frac{\mu_0 \mathcal{V}}{2} h^2_{\vec{k},\lambda}(t)
\end{aligned}$$

Analogy with the quantum harmonic oscillator

The analogy with the single harmonic oscillator (SHO) is not accidental: Electromagnetic radiation is coupled oscillation of the E and B fields

Classical SHO	Classical EM Modes
$\frac{d}{dt}x(t) = \frac{p(t)}{m}$	$\frac{d}{dt}e_{\vec{k},\lambda}(t) = \frac{k}{\epsilon_0}h_{\vec{k},\lambda}(t)$
$\frac{d}{dt}p(t) = -m\omega_0^2 x(t)$	$\frac{d}{dt}h_{\vec{k},\lambda}(t) = -\frac{k}{\mu_0}e_{\vec{k},\lambda}(t)$
$\mathcal{E} = \frac{p^2}{2m} + \frac{m\omega_0^2 x^2}{2}$	$\mathcal{E}_{\vec{k},\lambda} = \frac{\epsilon_0 \mathcal{V}}{2}e^2(t)_{\vec{k},\lambda} + \frac{\mu_0 \mathcal{V}}{2}h^2_{\vec{k},\lambda}(t)$

Electromagnetic field quantization

$$\hat{H}_{\vec{k},\lambda} = \frac{\epsilon_0 \mathcal{V}}{2}\hat{e}^2_{\vec{k},\lambda} + \frac{\mu_0 \mathcal{V}}{2}\hat{h}^2_{\vec{k},\lambda}$$

Hamiltonian for single-mode quantum radiation

Let us now introduce both creation and annihilation operators

$$\hat{a}_{\vec{k},\lambda} = \sqrt{\frac{\epsilon_0 \mathcal{V}}{2\hbar\omega_k}} \left(\hat{e}_{\vec{k},\lambda} + i\sqrt{\frac{\mu_0}{\epsilon_0}} \hat{h}_{\vec{k},\lambda} \right) \qquad \hat{a}^{\dagger}_{\vec{k},\lambda} = \sqrt{\frac{\epsilon_0 \mathcal{V}}{2\hbar\omega_k}} \left(\hat{e}_{\vec{k},\lambda} - i\sqrt{\frac{\mu_0}{\epsilon_0}} \hat{h}_{\vec{k},\lambda} \right)$$

Following the same procedure as the one use for the quantum harmonic oscillator, we show that

$$\hat{H}_{\vec{k},\lambda} = \hbar\omega_k \left[\hat{a}^{\dagger}_{\vec{k},\lambda} \hat{a}_{\vec{k},\lambda} + \frac{1}{2} \right]$$

Eigenstates $|n_{\vec{k},\lambda}\rangle$ with n=0,1,2,… corresponds to the number of photons into the mode

Even there are no photons in the mode, there is still a finite energy (i.e. vacuum) of energy $\frac{\hbar\omega_k}{2}$

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Multimode Hamiltonian

Since there are many modes in free space, the total Hamiltonian can be written as the sum of the individual modes. For convenience we label each mode (k,λ) with j

$$\hat{H}_{EM} = \sum_j \hbar\omega_j \left[\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2}\right]$$

Note that different modes do not interact with each other, i.e., each mode is independent

Eigenstates $|\{n\}\rangle = |n_1, n_2, \ldots, n_j, \ldots\rangle = |n_1\rangle\,|n_2\rangle \ldots |n_j\rangle \ldots$

with $E_{\{n\}} = \sum_j \hbar\omega_j (n_j + \frac{1}{2})$

And we do still have creation / annihilation operators (not Hermitian)

$$\hat{a}_j\,|n_j\rangle = \sqrt{n_j}\,|n_j - 1\rangle \text{ for } n_j > 0,\ \hat{a}_j\,|0\rangle = 0$$

$$\hat{a}_j^\dagger\,|n_j\rangle = \sqrt{n_j + 1}\,|n_j + 1\rangle$$

The vacuum state

Recall that in the quantum harmonic oscillator, the ground state (n = 0), is such that ⟨x⟩ = ⟨p⟩ = 0 but Δx Δp = ħ/2 . In quantum electrodynamics, it can be shown that for the vacuum state of each mode, ⟨e⟩ = ⟨h⟩ = 0

$$\Delta e^2 = \frac{\hbar\omega_k}{2\epsilon_0 \mathcal{V}} \qquad \Delta h^2 = \frac{\hbar\omega_k}{2\mu_0 \mathcal{V}} \quad \Rightarrow \quad \Delta e \Delta h = \frac{\hbar\omega_k c}{2\mathcal{V}}$$

There are zero-point fluctuations of the fields in vacuum which contribute to the finite zero-point energy and which can be thought to induce spontaneous emission

Total energy of the vacuum

$$E_0 = \frac{1}{2}\sum_j \hbar\omega_j \to \infty$$

However, the energy difference with excited states, which is what is typically observed, is finite

The vacuum state

The vacuum is responsible for remarkable features of quantum physics

The vacuum is the minimum dispersion state that is to say a state in which the fluctuations have the minimum values compatible with Heisenberg relationship

Explain the decay of an atom down to ground state by spontaneous emission

Affect the positions of the energy levels of the atom (Lamb shift)

PHYSICAL REVIEW VOLUME 72, NUMBER 3 AUGUST 1, 1947

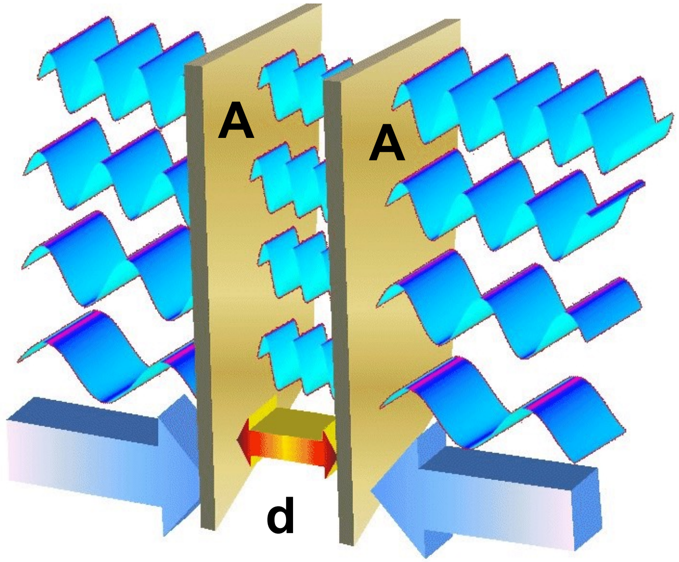
Fine Structure of the Hydrogen Atom by a Microwave Method* **

WILLIS E. LAMB, JR. AND ROBERT C. RETHERFORD
Columbia Radiation Laboratory, Department of Physics, Columbia University, New York, New York

The Casimir effect that is to say the attraction between two metallic plates close to each other

The Casimir effect

H. Casimir first predicted in 1948 that when two mirrors face each other in vacuum, fluctuations in the vacuum exert radiation pressure on them



Casimir force

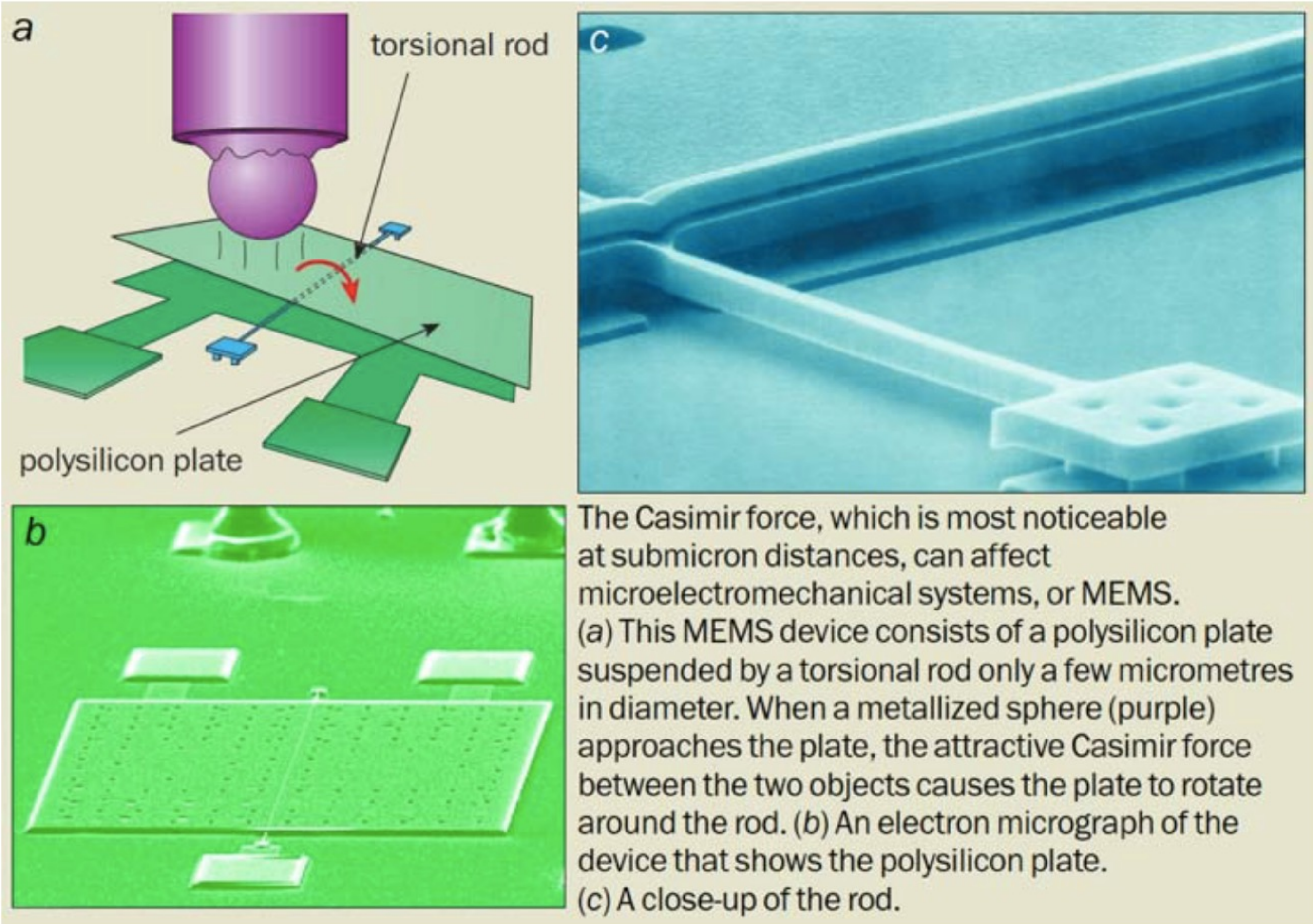
$$F_c = \frac{-\pi^2 \hbar c A}{240 d^4}$$

Since the space between two plates is different from the space outside, the vacuum fluctuations are also different in the two regions. The fluctuations exert different forces on the plates from inside and outside, resulting in a net pressure

Casimir forces set fundamental limits on the performance and the possible density of devices that can be optimized on a single chip

The Casimir effect

At the nanoscale, the Casimir force can produce a collapse of movable element to the substrate or the collapse of neighboring components during nanoscale device operation



The Casimir force, which is most noticeable at submicron distances, can affect microelectromechanical systems, or MEMS. (*a*) This MEMS device consists of a polysilicon plate suspended by a torsional rod only a few micrometres in diameter. When a metallized sphere (purple) approaches the plate, the attractive Casimir force between the two objects causes the plate to rotate around the rod. (*b*) An electron micrograph of the device that shows the polysilicon plate. (*c*) A close-up of the rod.

Science, Vol. 291 no. 5510, pp. 1941-1944, 2001

Electron-photon interaction

Alongside any quantum electronic system (hydrogen atom, potential well, etc.), there is also a quantum electromagnetic system. We can consider the composite quantum of an electron in some potential V(r) with the omnipresent electromagnetic field as the sum of the individual Hamiltonians with an interaction Hamiltonian

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + V(r)}_{\hat{H}_e} + \underbrace{\sum_j \hbar\omega_j \left[\hat{a}_j^\dagger \hat{a}_j + \frac{1}{2}\right]}_{\hat{H}_{EM}} - \underbrace{e\vec{E}\cdot\vec{r}}_{\hat{H}_{int}}$$

with $\vec{E} = \sum_j \vec{\lambda}_j \sqrt{\frac{\hbar\omega_j}{2\epsilon_0 \mathcal{V}}}(\hat{a}_j + \hat{a}_j^\dagger)$

leading to $\hat{H}_{int} = -e\sum_j \sqrt{\frac{\hbar\omega_j}{2\epsilon_0 \mathcal{V}}}(\hat{a}_j + \hat{a}_j^\dagger)\vec{\lambda}_j \cdot \vec{r}$

Eigenstates are linear combinations of |ψ$_i$,{n}⟩

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Electron-photon interaction

The interaction has a spatially dependent part which acts on the electron wave function and a photon operator part which acts on the photon states

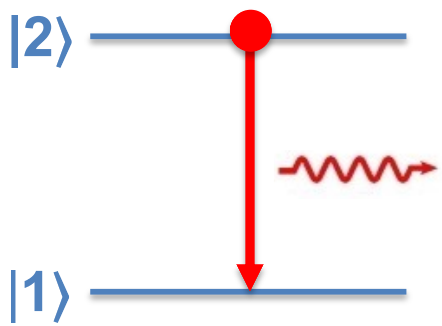
$$\langle \phi, \{m\} | \hat{H}_{int} | \psi, \{n\} \rangle = -e \sum_j \sqrt{\frac{\hbar\omega_j}{2\epsilon_0 \mathcal{V}}} \underbrace{\left\langle \phi \middle| \vec{\lambda}_j \cdot \vec{r} \middle| \psi \right\rangle}_{\text{Wavefunction}} \underbrace{\left\langle \{m\} \middle| \hat{a}_j + \hat{a}_j^\dagger \middle| \{n\} \right\rangle}_{\text{Photons}}$$

Suppose states $|1\rangle=|\psi_1,\{n_1\}\rangle$ and $|2\rangle=|\psi_2,\{n_2\}\rangle$ where $|\{n_1\}\rangle=|n_1,\ldots n_k,\ldots\rangle$ and $|\{n_2\}\rangle=|n_1,\ldots n_{k-1},\ldots\rangle$ with energy $E_{\psi 1}-E_{\psi 2}=\hbar\omega_k$

$$\left\langle 2 \middle| \hat{H}_{int} \middle| 1 \right\rangle = -e \sum_j \sqrt{\frac{\hbar\omega_j}{2\epsilon_0 \mathcal{V}}} \left\langle \{n_2\} \middle| (\hat{a}_j + \hat{a}_j^\dagger) \middle| \{n_1\} \right\rangle \left\langle \psi_2 \middle| \vec{\lambda}_j \cdot \vec{r} \middle| \psi_1 \right\rangle$$

$$= -e \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 \mathcal{V}}} \left\langle n_k + 1 \middle| \hat{a}_k^\dagger \middle| n_k \right\rangle \left\langle \psi_2 \middle| \vec{\lambda}_k \cdot \vec{r} \middle| \psi_1 \right\rangle$$

$$= -e \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 \mathcal{V}}} \sqrt{n_k + 1} \left\langle \psi_2 \middle| \vec{\lambda}_k \cdot \vec{r} \middle| \psi_1 \right\rangle$$



Transition I2> to I1> takes place while increasing the number of photons in mode k by 1 (a photon is emitted)

Electron-photon interaction

The interaction has a spatially dependent part which acts on the electron wave function and a photon operator part which acts on the photon states

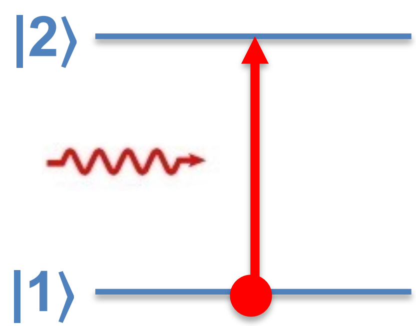
$$\langle \phi, \{m\} | \hat{H}_{int} | \psi, \{n\} \rangle = -e \sum_j \sqrt{\frac{\hbar\omega_j}{2\epsilon_0 \mathcal{V}}} \underbrace{\left\langle \phi \middle| \vec{\lambda}_j \cdot \vec{r} \middle| \psi \right\rangle}_{\textbf{Wavefunction}} \underbrace{\left\langle \{m\} \middle| \hat{a}_j + \hat{a}_j^{\dagger} \middle| \{n\} \right\rangle}_{\textbf{Photons}}$$

Suppose states $|1\rangle = |\psi_1, \{n_1\}\rangle$ and $|2\rangle = |\psi_2, \{n_2\}\rangle$ where $|\{n_1\}\rangle = |n_1, \ldots n_k, \ldots\rangle$ and $|\{n_2\}\rangle = |n_1, \ldots n_{k-1}, \ldots\rangle$ with energy $E_{\psi 2} - E_{\psi 1} = \hbar\omega_k$

$$\left\langle 2 \middle| \hat{H}_{int} \middle| 1 \right\rangle = -e \sum_j \sqrt{\frac{\hbar\omega_j}{2\epsilon_0 \mathcal{V}}} \left\langle \{n_2\} \middle| (\hat{a}_j + \hat{a}_j^{\dagger}) \middle| \{n_1\} \right\rangle \left\langle \psi_2 \middle| \vec{\lambda}_j \cdot \vec{r} \middle| \psi_1 \right\rangle$$

$$= -e \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 \mathcal{V}}} \langle n_k - 1 | \hat{a}_k | n_k \rangle \left\langle \psi_2 \middle| \vec{\lambda}_k \cdot \vec{r} \middle| \psi_1 \right\rangle$$

$$= -e \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 \mathcal{V}}} \sqrt{n_k} \left\langle \psi_2 \middle| \vec{\lambda}_k \cdot \vec{r} \middle| \psi_1 \right\rangle$$



Transition I1> to I2> takes place while decreasing the number of photons in mode k by 1 (a photon is absorbed)

Electron-photon interaction

The interaction has a spatially dependent part which acts on the electron wave function and a photon operator part which acts on the photon states

$$\langle \phi, \{m\} | \hat{H}_{int} | \psi, \{n\} \rangle = -e \sum_j \sqrt{\frac{\hbar \omega_j}{2\epsilon_0 \mathcal{V}}} \underbrace{\left\langle \phi \middle| \vec{\lambda}_j \cdot \vec{r} \middle| \psi \right\rangle}_{\text{Wavefunction}} \underbrace{\left\langle \{m\} \middle| \hat{a}_j + \hat{a}_j^\dagger \middle| \{n\} \right\rangle}_{\text{Photons}}$$

Rate of absorption $\left| \left\langle 2 \middle| \hat{H}_{int} \middle| 1 \right\rangle \right|^2 \propto n_k$

Rate of transitions $\left| \left\langle 2 \middle| \hat{H}_{int} \middle| 1 \right\rangle \right|^2 \propto n_k + 1$

And spontaneous emission is included

Two-state coupled to a single mode

Suppose a two-level electronic system coupled to only a single photon mode j (an example is an atom in a microscopic waveguide cavity)

$$H = \begin{pmatrix} E_a & 0 \\ 0 & E_b \end{pmatrix} + \hbar\omega_j (a_j^\dagger a_j + 1/2) + \hbar \begin{pmatrix} 0 & p \\ p^* & 0 \end{pmatrix} (\hat{a}_j + \hat{a}_j^\dagger)$$

With eigenstates such as $|\psi\rangle = \sum_{n=0}^{\infty} c_{a,n} |a, n\rangle + c_{b,n} |b, n\rangle$

Rotating wave approximation: Suppose the mode frequency is such that $\hbar\omega_j = E_a - E_b$ with $E_a > E_b$. Then we expect photon absorption to dominate the coupling from state b to a (p term) and emission to dominate the coupling from state a to b (p* term)

$$H = \begin{pmatrix} E_a & 0 \\ 0 & E_b \end{pmatrix} + \hbar\omega_j (a_j^\dagger a_j + 1/2) + \hbar \begin{pmatrix} 0 & p \\ 0 & 0 \end{pmatrix} \hat{a}_j + \hbar \begin{pmatrix} 0 & 0 \\ p^* & 0 \end{pmatrix} \hat{a}_j^\dagger$$

Two-state coupled to a single mode

The interaction Hamiltonian only couples states |a,n⟩ and |b,n+1⟩ to each other. So let us consider the action of the Hamiltonian just on the basis |a, n⟩ and |b, n+1⟩

$$H = \begin{pmatrix} E_a & 0 \\ 0 & E_b \end{pmatrix} + \hbar\omega_j \begin{pmatrix} n+(1/2) & 0 \\ 0 & n+(3/2) \end{pmatrix} + \begin{pmatrix} 0 & p\sqrt{n+1} \\ p^\dagger\sqrt{n+1} & 0 \end{pmatrix}$$

$$= \begin{pmatrix} E_D & p\sqrt{n+1} \\ p^\dagger\sqrt{n+1} & E_D \end{pmatrix}$$

with $E_D = E_a + \hbar\omega_j(n+1/2)$

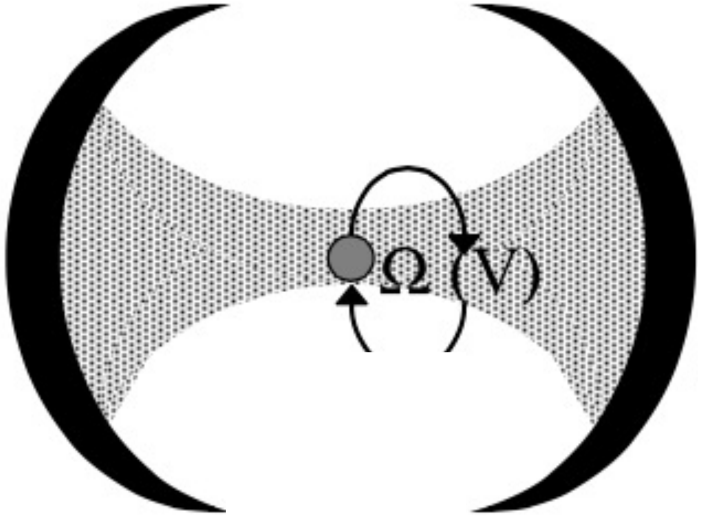
Eigenstates $E = E_D \pm |p|\sqrt{n+1}$ $\qquad \frac{1}{\sqrt{2}}(|a,n\rangle \pm |b,n+1\rangle)$

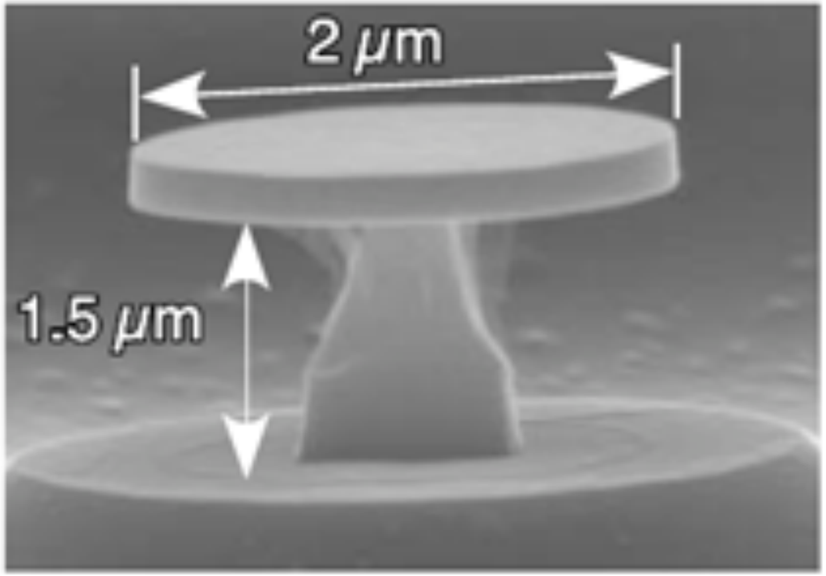
If the system starts out in, say, |a, n⟩, the state will Rabi oscillate back and forth between |b, n+1⟩, continuously emitting and reabsorbing a single photon

Rabi oscillations

Single localized emitter, initially in its excited state and resonantly coupled to a single empty mode of a lossless micro-cavity

No dissipation (e.g. perfect micro-cavity)





J. M Gerard, Single Quantum Dots, Topics Appl. Phys. 90, pp. 269–315 (2003)

Two-state coupled to a continuum

Suppose we have a two-level electronic system with states |a⟩ and |b⟩ in free space. The total Hamiltonian becomes (dropping the vacuum energy which just adds a global constant)

$$H = \begin{pmatrix} \hbar\omega_a & 0 \\ 0 & \hbar\omega_b \end{pmatrix} + \sum_j \hbar\omega_j a_j^\dagger a_j + \hbar \sum_j \begin{pmatrix} 0 & p_j \\ p_j^* & 0 \end{pmatrix} (\hat{a}_j + \hat{a}_j^\dagger)$$

Suppose the system starts in the state |a,{0}⟩ (i.e., in the upper electronic state with vacuum fluctuations). An excited state is not a stationary state so what is its time evolution?

The true eigenstates of H are complicated, so we write the state of the system in the basis of |a, {n}⟩ and |b, {n}⟩. Because these are not energy eigenstates anymore, we must allow their coefficients to be time-dependent

Two-state coupled to a continuum

Suppose we have a two-level electronic system with states |a⟩ and |b⟩ in free space. The total Hamiltonian becomes (dropping the vacuum energy which just adds a global constant)

$$H = \begin{pmatrix} \hbar\omega_a & 0 \\ 0 & \hbar\omega_b \end{pmatrix} + \sum_j \hbar\omega_j a_j^\dagger a_j + \hbar \sum_j \begin{pmatrix} 0 & p_j \\ p_j^* & 0 \end{pmatrix} (\hat{a}_j + \hat{a}_j^\dagger)$$

Suppose the system starts in the state |a,{0}⟩ (i.e., in the upper electronic state with vacuum fluctuations). An excited state is not a stationary state so what is its time evolution?

Since the p_j interaction only couples |a,{0}⟩ to states |b,{1j}⟩ (product state of |b⟩ with one photon in mode j), we only need to consider these states in our expansion

$$|\psi(t)\rangle = c_{a,\{0\}}(t) e^{-i\omega_a t} |a, \{0\}\rangle + \sum_j c_{b,\{1_j\}}(t) e^{-i(\omega_b+\omega_j)t} |b, 1_j\rangle$$

Two-state coupled to a continuum

Substituting into the time-dependent Schrödinger equation, we obtain

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\left[c_{a,\{0\}}(t)e^{-i\omega_a t}\,|a,\{0\}\rangle + \sum_j c_{b,\{1_j\}}(t)e^{-i(\omega_b+\omega_j)t}\,|b,1_j\rangle\right] = 0$$

Working out the results of the time-dependent Schrödinger equation and then projecting onto |a, {0}⟩ and |b, {1j}⟩, we get

$$\dot{c}_{a,\{0\}}(t) = -i\sum_j p_j e^{-i(\omega_j-\Delta)t} c_{b,\{1_j\}}(t)$$

$$\dot{c}_{b,\{1_j\}}(t) = -ip_j^* e^{i(\omega_j-\Delta)t} c_{a,\{0\}}(t)$$

With the frequency detuning $\Delta = \omega_a - \omega_b$

Two-state coupled to a continuum

We can integrate the second equation from t = 0 to t, recalling our initial condition $c_{b,\{1j\}} = 0$, and then substitute in the first equation to obtain

$$\dot{c}_{a,\{0\}}(t) = -\sum_j |p_j|^2 \int_0^t e^{-i(\omega_j - \Delta)t'} c_{a,\{0\}}(t')dt'$$

$$\sum_j \to \int dE_j g(E_j)$$

Density of photons

Summation on a continuous range of photons mode j

$$\dot{c}_{a,\{0\}}(t) \simeq -|p_j|^2 c_{a,\{0\}}(t)\hbar \int d\omega_j g(\hbar\omega_j) \int_0^t e^{-i(\omega_j - \Delta)t'} dt'$$

The above equation assumes that $c_{a,\{0\}}$ changes slowly with time, such that $c_{a,\{0\}}(t') \approx c_{a,\{0\}}(t)$

Two-state coupled to a continuum

What is the long time limit of this?

$$\lim_{t\to\infty}\int_0^t dt' e^{-i(\omega-\Delta)t} = \pi\delta(\omega-\Delta)$$

leading to

$$\dot{c}_{a,\{0\}}(t) = -\frac{\pi}{\hbar}|p_j|^2 c_{a,\{0\}}(t)\int dE_j g(\hbar\omega_j)\delta(\hbar\omega - \hbar\Delta)$$

$$\dot{c}_{a,\{0\}}(t) = -\frac{\Gamma}{2}c_{a,\{0\}}(t) \qquad \rightarrow c_{a,\{0\}} = \exp(-\Gamma t/2)$$

The integration of this very last equation allows to retrieve the so-called Fermi-Golden rule

Two-state coupled to a continuum

The probability of the system remaining in its initially excited electronic state without emitting a photon is given by

$$|c_{a,\{0\}}|^2 = \exp(-\Gamma t)$$

i.e.

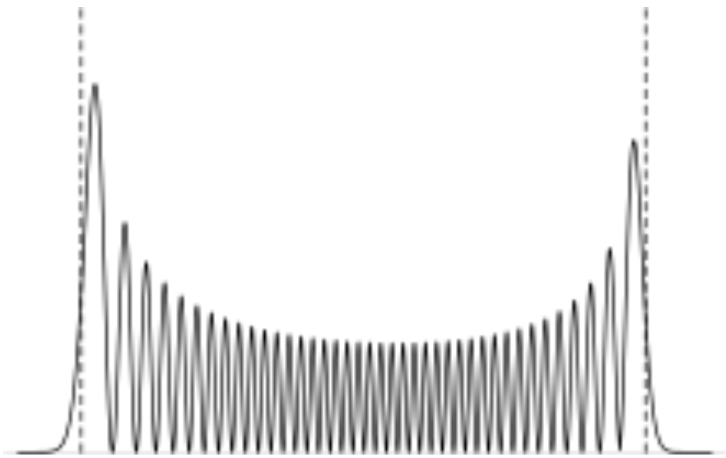
$$\Gamma = \frac{2\pi}{\hbar}|p_j|^2 g(\hbar(\omega_a - \omega_b))$$

which is the so-called Fermi golden rule

In other words, the system irreversibly transitions away from its initial excited state by emitting a photon; substituting in values for p_j and the photon DOS, we obtain exactly the spontaneous emission rate predicted by the Einstein relation and previously calculated semi-classically

Section 13

The WKB Approximation



Further material on perturbation theories is available in the supplementary information documents II and III

WKB approximation

WKB=Wentzel-Kramers-Brillouin is a way to semi-classically approximate wave functions for slowly varying V(x)

We write a general wave function $\psi(x) = Ae^{iS(x)/\hbar}$ where A is real and S(x) is a complex function

Substituting $\psi(x)$ into the Schrödinger's equation, we get

$$-i\hbar\frac{\partial^2 S(x)}{\partial x^2} + \left(\frac{\partial S(x)}{\partial x}\right)^2 = p^2(x)$$

$$p(x) = \sqrt{2m(E - V(x))} \equiv \hbar k(x)$$

Now expand S(x) in powers of $\hbar$ such that

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{\hbar^2}{2}S_2(x) + \cdots$$

WKB approximation

Using the series expansion of S(x) we find

$$0 = \left[\left(\frac{\partial S_0(x)}{\partial x}\right)^2 - p^2(x)\right] + 2\hbar\left[\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} - \frac{i}{2}\frac{\partial^2 S_0(x)}{\partial x^2}\right] +$$

$$\hbar^2\left[\frac{\partial S_0}{\partial x}\frac{\partial S_2}{\partial x} + \left(\frac{\partial S_1(x)}{\partial x}\right)^2 - i\frac{\partial^2 S_0(x)}{\partial x^2}\right] + \mathcal{O}(\hbar^3)$$

Every term of the series in $\hbar$ must vanish, i.e.,

$$\left(\frac{\partial S_0(x)}{\partial x}\right)^2 = p^2(x)$$

$$\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} = \frac{i}{2}\frac{\partial^2 S_0(x)}{\partial x^2}$$

$$\frac{\partial S_0}{\partial x}\frac{\partial S_2}{\partial x} + \left(\frac{\partial S_1(x)}{\partial x}\right)^2 = i\frac{\partial^2 S_0(x)}{\partial x^2}$$

WKB approximation

We can solve the equations sequentially

$$S_0(x) = \pm \int_{x_0}^{x} p(x')dx' = \pm\hbar \int_{x_0}^{x} k(x')dx'$$

$$S_1(x) = \frac{i}{2}\ln\left(\frac{\partial S_0}{\partial x}\right) = \frac{i}{2}\ln(\hbar k(x))$$

Substituting $S_0 + \hbar S_1$ **in** ψ **and absorbing integration constants in A**

$$\psi(x) \approx Ak^{-1/2}(x)\exp\left(\pm i\int^{x} k(x')dx'\right) \quad \text{for } E>V(x)$$

$$\psi(x) \approx A\kappa^{-1/2}(x)\exp\left(\pm \int^{x} \kappa(x')dx'\right) \quad \text{for } E<V(x)$$

where $\kappa = \sqrt{2m(V(x)-E)/\hbar^2}.$

WKB approximation

Let $V(x) = m\omega x^2/2$ with classical tuning point such $x_0 = \pm\sqrt{\frac{2E}{m\omega^2}}$

$$\int_{x_1}^{x_2} k dx = \int_{-x_0}^{x_0} \sqrt{\frac{2m(E - m\omega x^2/2)}{\hbar^2}} dx$$

$$= \sqrt{\frac{2mE}{\hbar^2}} \int_{-x_0}^{x_0} \sqrt{1 - \frac{x^2}{x_0^2}} dx$$

$$= \sqrt{\frac{2mE}{\hbar^2}} x_0 \int_0^{\pi} \sqrt{1 - \cos^2\theta} \sin\theta d\theta$$

$$= \frac{2E}{\hbar\omega}\frac{\pi}{2} = (n - \frac{1}{2})\pi$$

for $n = 1, 2, 3, \ldots$ this implies $E = \hbar\omega(n + \frac{1}{2})$ for $n = 0, 1, 2 \ldots$

which coincides with the exact solution for the harmonic oscillator!
However, most of the time the WKB is not so exact….

WKB approximation

WKB approximation is valid when V(x) changes so slowly that the local momentum is constant over a few wavelengths

$$\frac{\lambda(x)}{4\pi}\left|\frac{dk(x)}{dx}\right| \ll k(x)$$

WKB approximation breaks down near the classical turning points because k(x) → 0 and λ → ∞ (connections formula required)

WKB is particularly useful for estimating tunneling rates and bound state energies. Since bound states imply standing waves, we require that

$$\int_{x_1}^{x_2} k(x)dx = \int_{x_1}^{x_2} \frac{\sqrt{2m(E-V(x))}}{\hbar}dx = n\pi + \delta\theta$$

where x_1, x_2 are the classical turning points, n is an integer, and $\delta\theta$ is an additional phase accounting for penetration of wave function into barrier

WKB approximation

In classically forbidden regions for which $V(x) > E$ we have

$$\psi(x) \approx \frac{A}{\sqrt{\kappa(x)}} \exp(\pm \int \kappa(x')dx')$$

where $\kappa(x) = \sqrt{\dfrac{2m(V(x)-E)}{\hbar^2}}$

We can estimate the tunneling probability through a classically forbidden region bounded by $[x_1, x_2]$ using

$$T = \left|\frac{\Psi(x_2)}{\Psi(x_1)}\right|^2 \simeq \exp\left(-2\int_{x_1}^{x_2} \kappa(x)dx\right)$$

In practice this equation is very helpful for estimating tunneling in real physical systems, including semiconductor devices

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