UFS Lecture 7: Review of Quantum Mechanics

Review of Quantum Mechanics
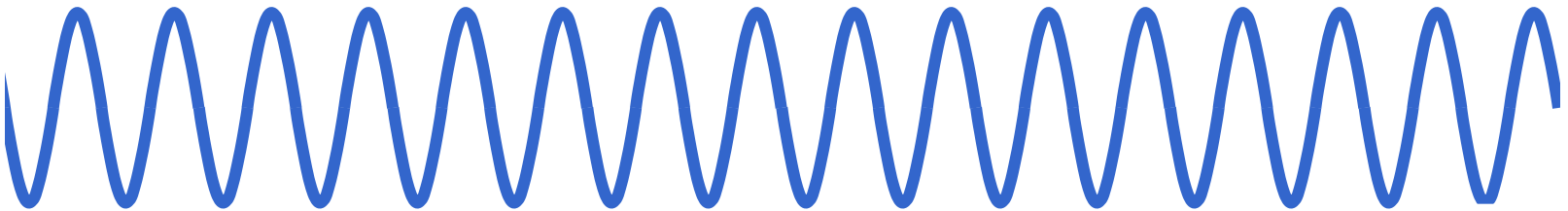
and

History of the Laser

Quantum mechanics: wave motion of a particle

In 1923, de Broglie (1892-1987) suggested that massive particles should have wave properties similar to electromagnetic radiation. The matter wave should also be a solution to a wave equation.

The solution should look like:
$$\Psi(x,t) = A \exp[j(kx - \omega t - \theta)]$$

Define the wave number k and the angular frequency ω as usual:
$$k = \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T}$$

Wave function and probability

The wave function $\Psi(\vec{r}, t)$ determines the likelihood (or probability) of finding a particle at a particular position in space at a given time:

$$\Psi(\vec{r}, t)$$

Probability amplitude for finding particle in volume element dV at position r at time t.

Enables to compute outcome of every possible experiment involving that system.

$$|\Psi(\vec{r}, t)|^2 \, dV$$

Probability of finding particle in volume element dV at position r at time t.

The Schrödinger wave equation

In classical mechanics, the particle state is determined by its position and momentum. The state evolution is determined by Newton's law.

In quantum mechanics the particle state is completely described by its wave function. The state is determined by the Schrödinger equation.

The Schrödinger wave equation for the wave function $\Psi\left(\vec{r}, t\right)$ for a particle in a potential V is:

$$ j\,\hbar\frac{\partial \Psi\left(\vec{r}, t\right)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\ \Psi\left(\vec{r}, t\right) + V\left(\vec{r}\right)\ \Psi\left(\vec{r}, t\right) $$

where $\quad \Delta = \nabla \cdot \nabla \equiv \nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}$

Time-independent (stationary) Schrödinger equation

$$\mathrm{j}\,\hbar\frac{\partial \Psi\left(\vec{r},t\right)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\,\Psi\left(\vec{r},t\right) + V\left(\vec{r}\right)\,\Psi\left(\vec{r},t\right)$$

Stationary states:

$$\Psi\left(\vec{r},t\right) = \psi\left(\vec{r}\right)\,e^{-\mathrm{j}\,\omega t}$$

Eigen frequency

Probability density is time independent:

$$\left|\Psi\left(\vec{r},t\right)\right|^2 = \left|\psi\left(\vec{r}\right)\right|^2 = \mathrm{const.}$$

Total energy of the system: $E = \hbar\omega$

Time-independent (stationary) Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\,\psi\left(\vec{r}\right) + V\left(\vec{r}\right)\,\psi\left(\vec{r}\right) = E\,\psi\left(\vec{r}\right)$$

Eigen energy

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Example: 1-d Infinite box potential
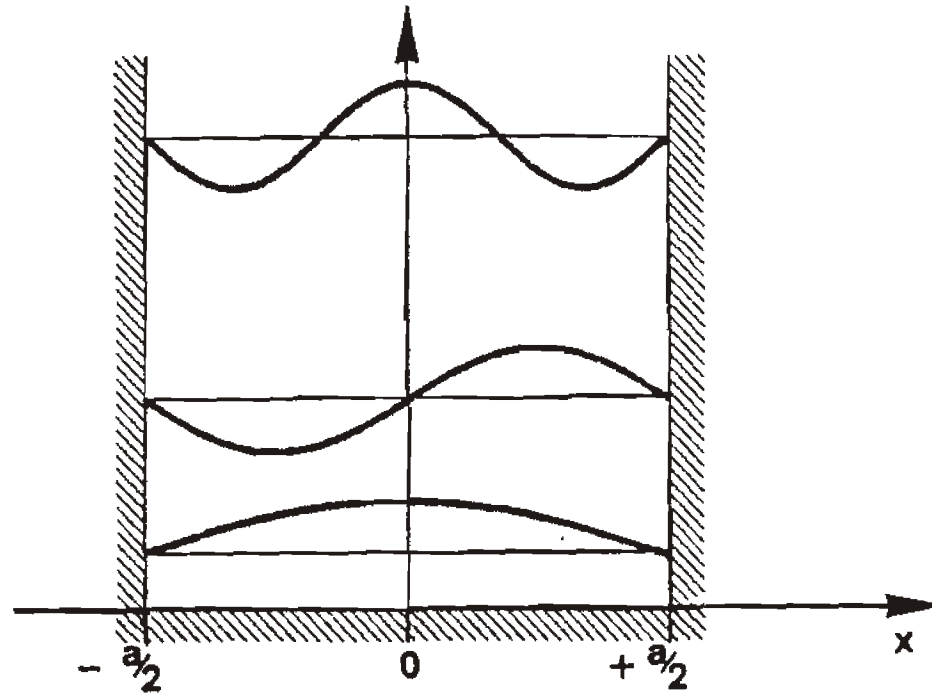
One dimensional box potential with infinite barriers.

$$V(x) = \begin{cases} 0, & \text{for } |x| < a/2 \\ \infty, & \text{for } |x| \geq a/2 \end{cases}$$

Example: 1-d Infinite box potential

Time-independent Schrödinger equation in the interval [-a/2, a/2]

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

For $|x| \geq a/2$ the wave function must vanish

$$\psi(x = \pm a/2) = 0$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\,\cos\,\frac{n\pi x}{a}\quad \text{for}\quad n = 1, 3, 5\ldots,$$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\,\frac{n\pi x}{a}\quad \text{for}\quad n = 2, 4, 6\ldots.$$

Energy eigenvalues: $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$

Example: 1-d Infinite box potential

Stationary states are orthogonal to each other

$$\int_{-\infty}^{+\infty} \psi_m (x)^* \psi_n (x) \, dx = \delta_{mn}$$

Form complete set:

$$f(x) = \sum_{n=0}^{\infty} c_n \psi_n (x)$$

With coefficient:

$$c_m = \int_{-a/2}^{a/2} \psi_m (x)^* f(x) \, dx$$

Quantum mechanics: wave mechanics

Physically measurable quantities = Observables

Observables are represented by Hermitian operators

$$\int \psi_n^* (x) \left(H_{op}\psi_m (x)\right) dx = \int \left(H_{op}\psi_n (x)\right)^* \psi_m (x)\, dx$$

Examples for one dimensional systems:

$$x \quad : \quad \text{position operator}$$

$$p \quad = \quad \frac{\hbar}{j}\frac{\partial}{\partial x} \; : \; \text{momentum operator}$$

$$H(p,x) \quad = \quad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \; : \; \text{Hamiltonian operator}$$

The wave function $\psi(x,t)$ allows us to compute the statistics of measurements of observables executed on the system in an ideal way, (the best you can do), without necessarily specifying the apparatus that does it.

Statistics for position, momentum, and energy

Position: x

$$\langle x \rangle \;=\; \int_{-\infty}^{\infty} \Psi^*(x,t)\; x\; \Psi(x,t)\; dx$$

Momentum: p

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\; \frac{\hbar}{\mathrm{j}}\frac{\partial}{\partial x}\; \Psi(x,t)\; dx$$

Energy: H

$$\langle H(x,p) \rangle \;=\; \int_{-\infty}^{\infty} \Psi^*(x,t)\; H(x,p)\; \Psi(x,t)\; dx$$
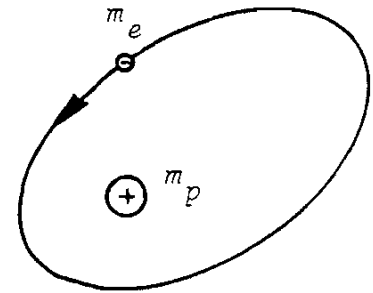
If the system is in an energy eigenstate, i.e.,

$$\Psi(x,t) \;=\; \psi_n(x)\; e^{\mathrm{j}\omega_n t} \qquad H(x,p)\,\psi_n(x) = E_n\,\psi_n(x)$$

$$\langle H(x,p) \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\; E_n\; \Psi(x,t)\; dx = E_n$$

Example: Hydrogen atom

Schrödinger eqn for H-atom:

$$\Delta\psi\left(\vec{r}\right) + \frac{2m_0}{\hbar^2}\left(E - V\left(\vec{r}\right)\right)\ \psi\left(\vec{r}\right) = 0$$

with

$$V\left(\vec{r}\right) = -\frac{e_0^2}{4\pi\,\varepsilon_0\,\left|\vec{r}\right|} \qquad \textbf{and} \qquad m_0 = \frac{m_p \cdot me}{m_p + m_e} \sim m_e$$

1836 x m_e

Laplace operator in spherical coordinates:

$$\Delta\psi = \frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\psi}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right]$$

Stationary Schrödinger eqn for H-atom:

$$\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial\psi}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2\psi}{\partial\varphi^2}\right] + \frac{2m_0}{\hbar^2}\left(E + \frac{e_0^2}{4\pi\,\varepsilon_0\,r}\right)\psi = 0$$

Hydrogen atom at ground state
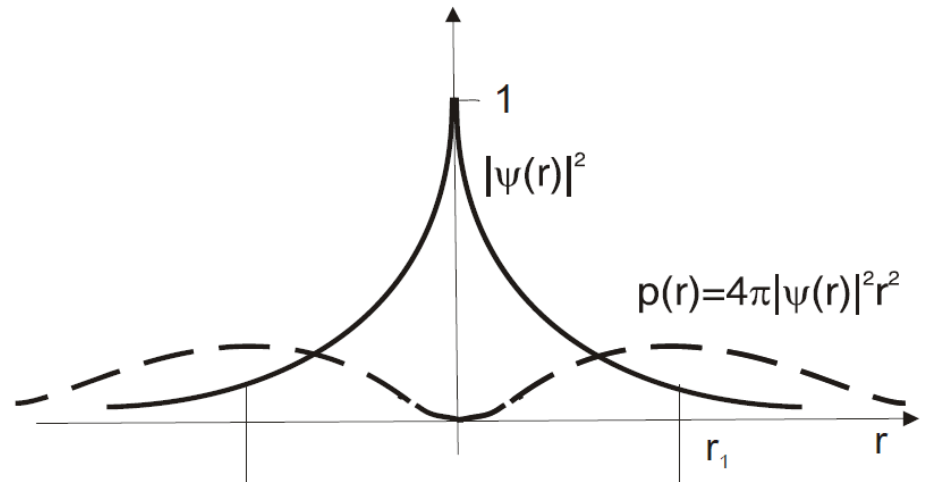
$$\psi(r, \vartheta, \varphi) = \psi_1(r)$$

leads to

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right]\psi_1(r) + \frac{2m_0}{\hbar^2}\left(E + \frac{e_0^2}{4\pi\varepsilon_0 r}\right)\psi_1(r) = 0$$

Ground state wave function:

$$\psi_1(r) = \sqrt{\frac{1}{\pi r_1^3}}e^{-r/r_1}$$

Bohr radius

$$r_1 = \frac{\varepsilon_0 h^2}{\pi e^2 m_0} \approx 0.529 \cdot 10^{-10} m$$

$|\psi(r)|^2$

$p(r) = 4\pi|\psi(r)|^2 r^2$

Ground state energy: $\qquad E_1 = \frac{\hbar^2}{2m_0 r_1^2} = -\frac{me^4}{8\varepsilon_0^2 h^2} = -13.53\text{eV}$

Hydrogen atom at excited states

Solve the Schrödinger eqn by separating variables:

$$\psi\left(r,\vartheta,\varphi\right) = R\left(r\right) \cdot Y\left(\vartheta,\varphi\right)$$

$$\left\{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R\right) + \frac{2m_0 r^2}{\hbar^2}\left(E + \frac{e_0^2}{4\pi\varepsilon_0 r}\right)\right\} = -\frac{1}{Y}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right)\right] + \frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2}$$

The left side of this equation is only a function of the radius r, and the right side of the angles ϑ and φ. Therefore, this equation can only be fulfilled if each side is equal to a constant number C, that is

$$\left\{\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R\right) + \frac{2m_0 r^2}{\hbar^2}\left(E + \frac{e_0^2}{4\pi\varepsilon_0 r}\right)\right\} = C$$

$$-\frac{1}{Y}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial Y}{\partial\vartheta}\right)\right] + \frac{1}{\sin^2\vartheta}\frac{\partial^2 Y}{\partial\varphi^2} = C$$

Hydrogen atom at excited states

Spherical Harmonics:

$$Y_1^m(\vartheta, \varphi) = (-1)^m \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}} \, P_1^m(\cos\vartheta) \, e^{jm\,\varphi}$$

Normalization Factor

Associated Legendre Polynomials

$l = 0, 1, 2, \ldots$ positive whole number

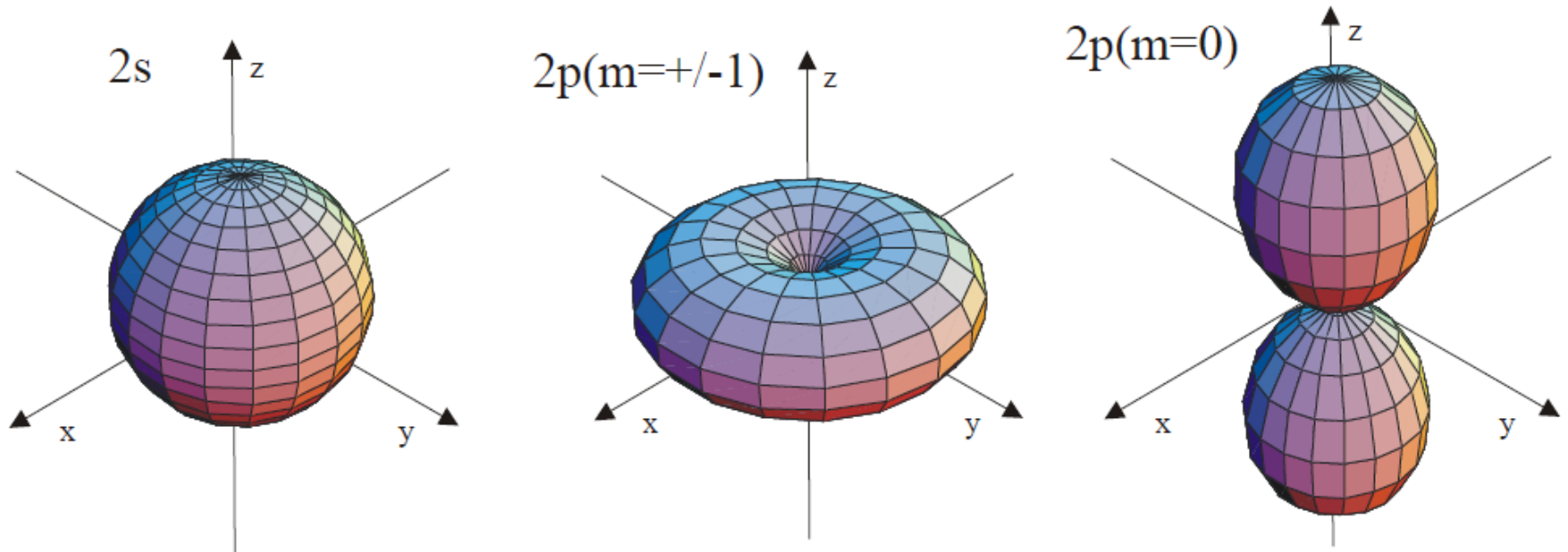$m = 0, \pm 1, \pm 2, \ldots, \pm l$ $\qquad C = l(l+1)$

Radial wave functions:

$$\frac{d^2 R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left(\frac{2m_0 E}{\hbar^2} + \frac{m_0 e_0^2}{2\pi\varepsilon_0 \hbar^2 r} - \frac{l(l+1)}{r^2}\right) R = 0$$

$$E = E_n = -\frac{m_0 e^4}{8\varepsilon_0^2 h^2}\frac{1}{n^2} \qquad R_{n1}(r) = \frac{2}{n^2}\sqrt{\frac{(n-l-1)!}{[(n+l)!]^3}} \, r_1^{-3/2} \cdot \rho^1 \, L_{n-l-1}^{21+1}(\rho) \, e^{-\rho/2}$$

Laguerre Polynomials

$n = 1, 2, \ldots$ and $n \geq l+1$ $\qquad \rho = \frac{2r}{nr_1}$

Hydrogen atom at excited states

Surfaces of constant probability density for the first three excited states (n=2) of the hydrogen atom.

Wave functions and quantum numbers

$$\psi_{nlm}(r, \vartheta, \varphi) = R_{nl}(r) \; Y_l^m(\vartheta, \varphi)$$

n: energy:

$$H\psi_{nlm}(\vec{r}) = E_n \psi_{nlm}(\vec{r})$$

l: angular momentum:

$$\vec{L}^2 \, \psi_{nlm}(r, \vartheta, \varphi) = l(l+1)\hbar^2 \, \psi_{nlm}(r, \vartheta, \varphi)$$

m: z-component of angular momentum:

$$L_z \, \psi_{nlm}(r, \vartheta, \varphi) = m\hbar \, \psi_{nlm}(r, \vartheta, \varphi)$$

s: spin of the electron:

$$s = \pm\hbar/2$$

Spin is an internal angular momentum of the electron that carries a magnetic moment with it.

n, l, m, s: complete set of quantum numbers to determine state uniquely!

Superposition states and radiative transitions

For energy eigen state:

$$\langle \vec{r} \rangle = \int_{-\infty}^{\infty} \vec{r} \, |\Psi(\vec{r},t)|^2 \, d^3\vec{r} = 0$$

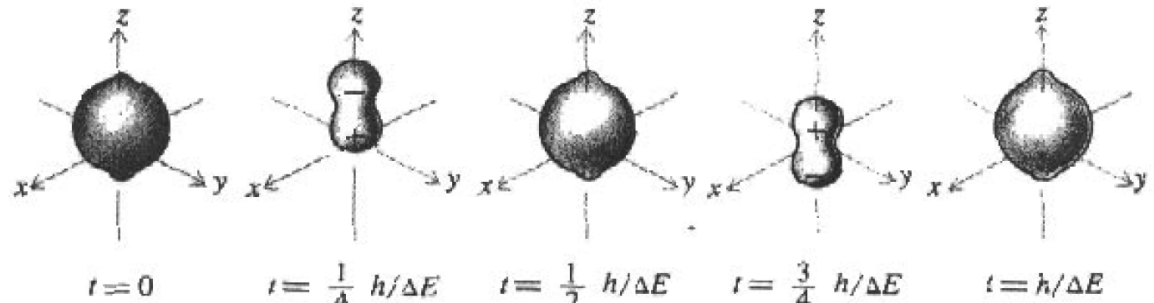$$\vec{p} = -e \langle \vec{r} \rangle \longrightarrow \ \ \mathbf{O}$$

Average dipole moment vanishes. Therefore the atom does not radiate in a stationary state as postulated in the Bohr model.
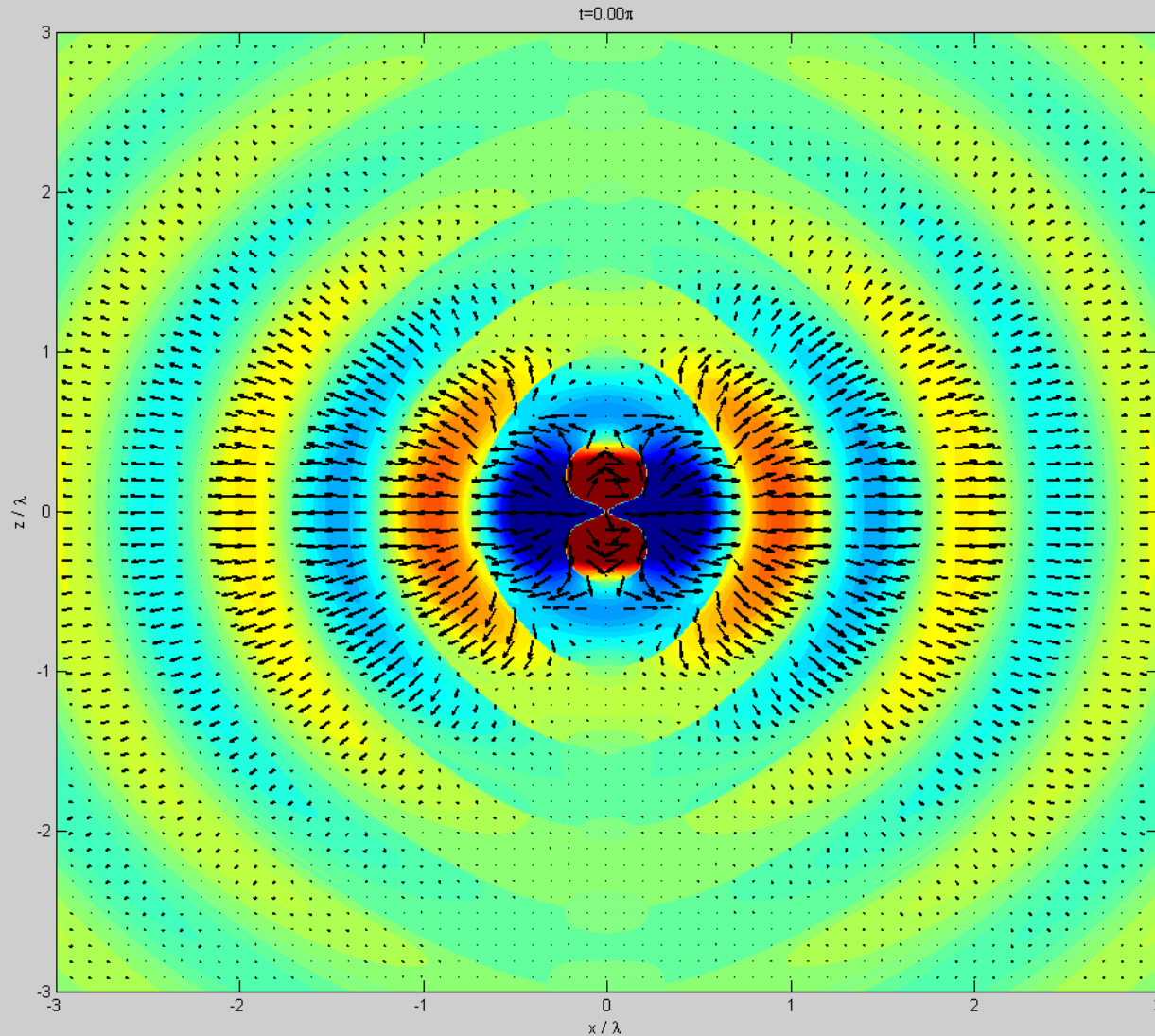
For superposition state: **1s + 2p (m=0)**

$$\frac{1}{\sqrt{2}} \left(\psi_{100}(\vec{r},t) + \psi_{210}(\vec{r},t) \right) = \frac{1}{\sqrt{2\pi}\sqrt{r_1^3}} \left(e^{-r/r_1} e^{-jE_1 t/\hbar} + \frac{1}{4\sqrt{2}} \frac{r}{r_1} e^{-r/2r_1} \cos\vartheta \, e^{-jE_2 t/\hbar} \right)$$

In the probability density (i.e. the magnitude square of the wave function), the contributions between the ground state and excited state interfer positively or negatively depending on the relative phase between the two wave functions, which depends on the phase angle $\Delta E t/\hbar$, with $\Delta E = E_2 - E_1$.

$$t=0 \qquad t=\tfrac{1}{4}\,h/\Delta E \qquad t=\tfrac{1}{2}\,h/\Delta E \qquad t=\tfrac{3}{4}\,h/\Delta E \qquad t=h/\Delta E$$

Oscillating dipole moment emits new EM wave at the oscillating frequency

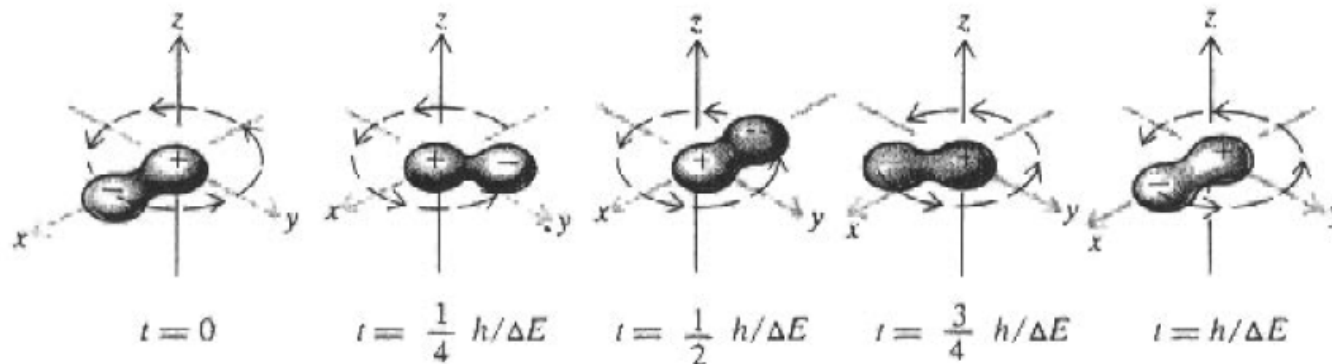**It does not emit in the oscillating direction!** *From wiki*

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Superposition states and radiative transitions

For superposition state: 1s + 2p (m=1)

Instead of an oscillating charge distribution, the atom shows now a rotating dipole, which emits a circular polarized electromagnetic wave.

$$\frac{1}{\sqrt{2}}\left(\psi_{1s}(\vec{r},t) + \psi_{2p,m=1}(\vec{r},t)\right) = \frac{1}{\sqrt{2}}\left(\psi_{100}(\vec{r},t) + \psi_{211}(\vec{r},t)\right)$$

$$= \frac{1}{\sqrt{2\pi}\sqrt{r_1^3}}\left(e^{-r/r_1}e^{-jE_1t/\hbar} + \frac{1}{8}\frac{r}{r_1}e^{-r/2r_1}\sin\vartheta e^{j\varphi}e^{-jE_2t/\hbar}\right)$$

$$t=0 \qquad t=\tfrac{1}{4}\,h/\Delta E \qquad t=\tfrac{1}{2}\,h/\Delta E \qquad t=\tfrac{3}{4}\,h/\Delta E \qquad t=h/\Delta E$$

Early history of lasers

- 1917: *on the quantum theory of radiation* – Einstein's paper

- 1954: MASER by Charles Townes (1915—2015) *et al*.

- 1957: LASER coined by Gordon Gould (1920-2005).

- 1958: Charles Townes (Nobel Prize in 1964) and Schawlow (Nobel Prize in 1981) conceive basic ideas for a laser.

- 1960: First laser (Ruby) by Maiman

August 6, 1960   N A T U R E   No. 4736   493
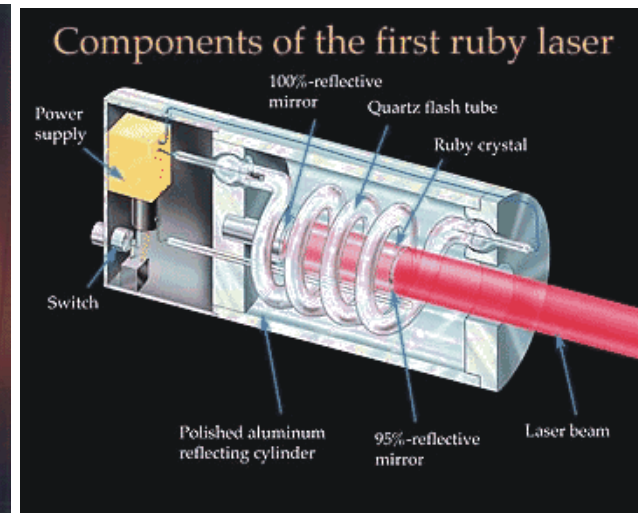
Stimulated Optical Radiation in Ruby

Schawlow and Townes[1] have proposed a technique for the generation of very monochromatic radiation in the infra-red optical region of the spectrum using an alkali vapour as the active medium. Javan[2] and Sanders[3] have discussed proposals involving electron-excited gaseous systems. In this laboratory an optical pumping technique has been successfully applied to a fluorescent solid resulting in the attainment of negative temperatures and stimulated optical emission at a wave-length of 6943 Å.; the active

T. H. MAIMAN

Hughes Research Laboratories,
A Division of Hughes Aircraft Co.,
Malibu, California.
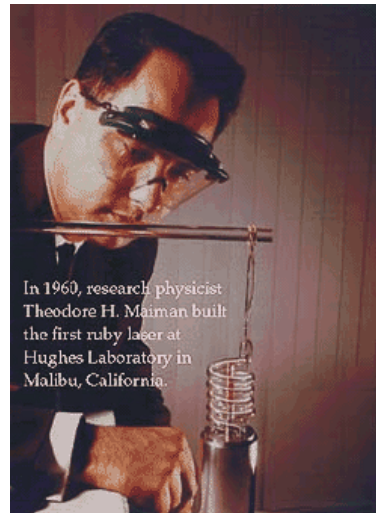
In 1960, research physicist Theodore H. Maiman built the first ruby laser at Hughes Laboratory in Malibu, California.

Components of the first ruby laser

Power supply — Switch — Polished aluminum reflecting cylinder — 100%-reflective mirror — Quartz flash tube — Ruby crystal — 95%-reflective mirror — Laser beam

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- 1958: Charles Townes (Nobel Prize in 1964) and Schawlow (Nobel Prize in 1981) conceive basic ideas for a laser.

- 1960: First laser (Ruby) by Maiman

- 1960: First HeNe laser by Ali Javan at Bell Labs

- 1961: Lasers (Ruby) first became commercially available

- 1962: First Semiconductor injection laser by Robert Hall at GE

- 1977: Gordon Gould awarded the patent for the laser.

Laser basics: three key elements

Continuous wave (CW) laser
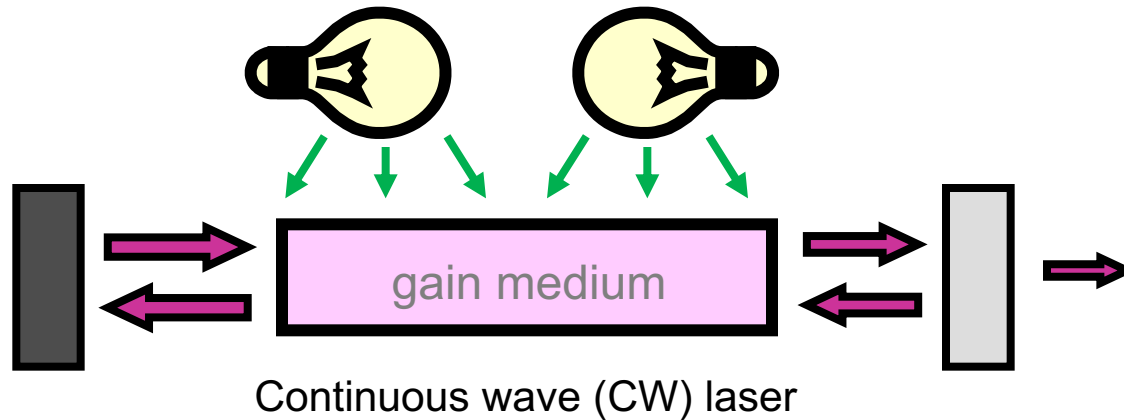
- **Gain medium**
  - Enable stimulated emission to produce identical copies of photons
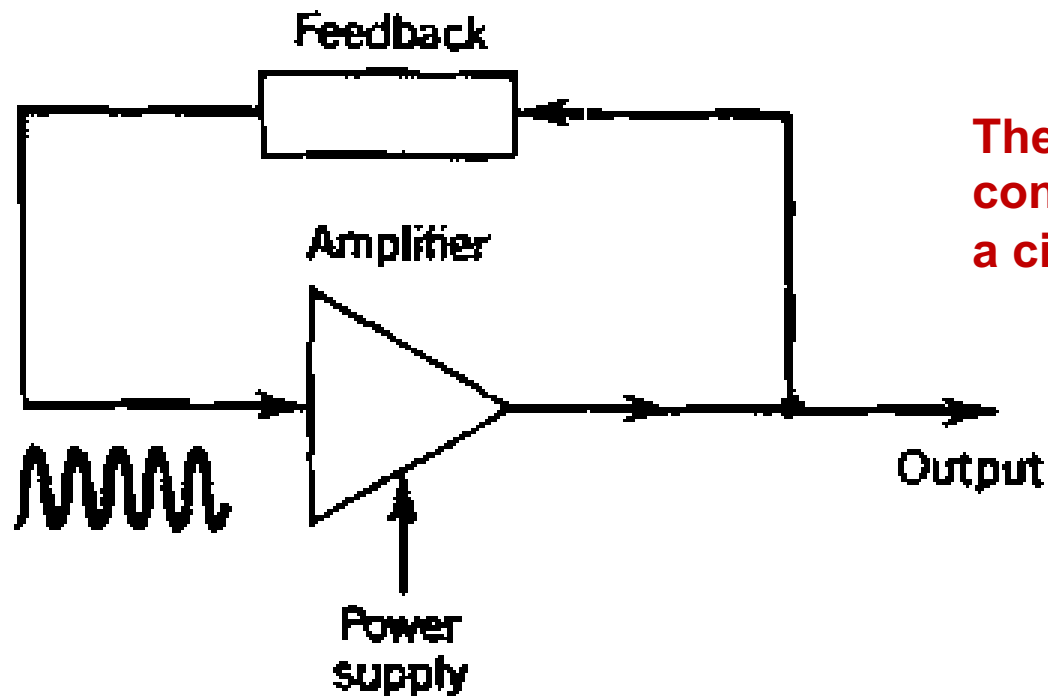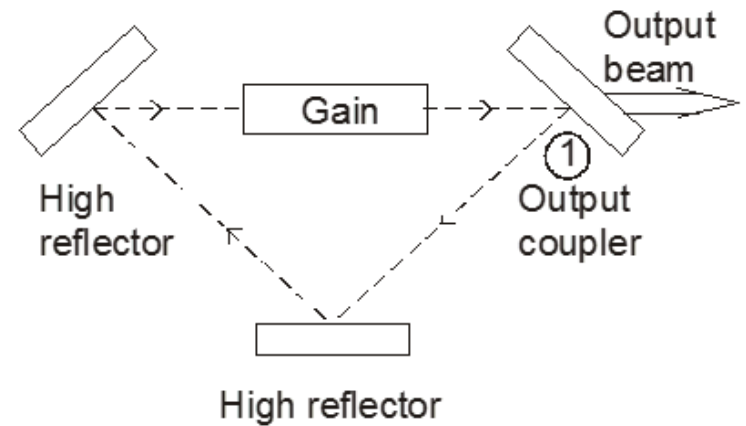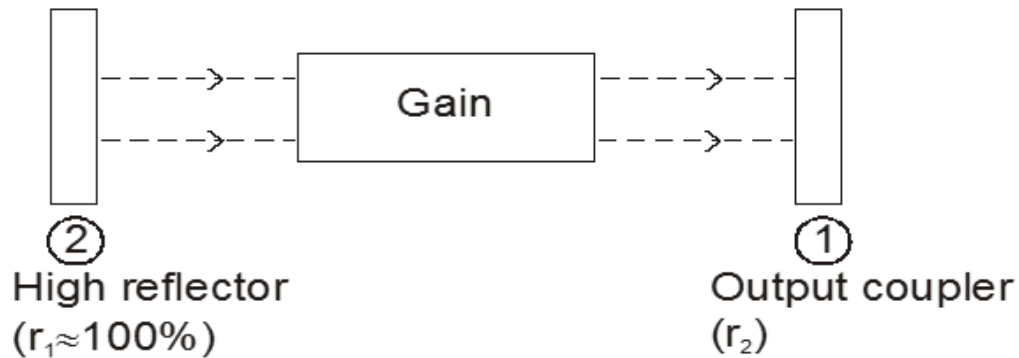 - Determine the light wavelength

- **Pump**
  - Inject power into the gain medium
  - Achieve population inversion

- **Resonator cavity**
  - make light wave oscillating to efficiently extract energy stored in the gain medium
  - Improve directionality and color purity of the light
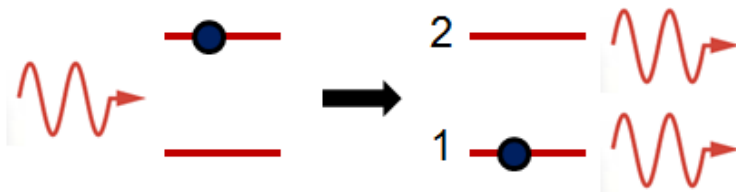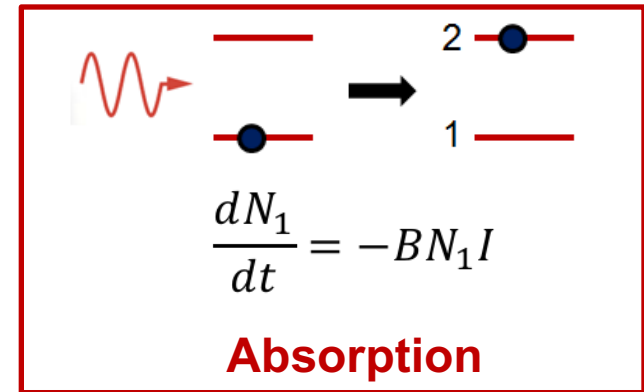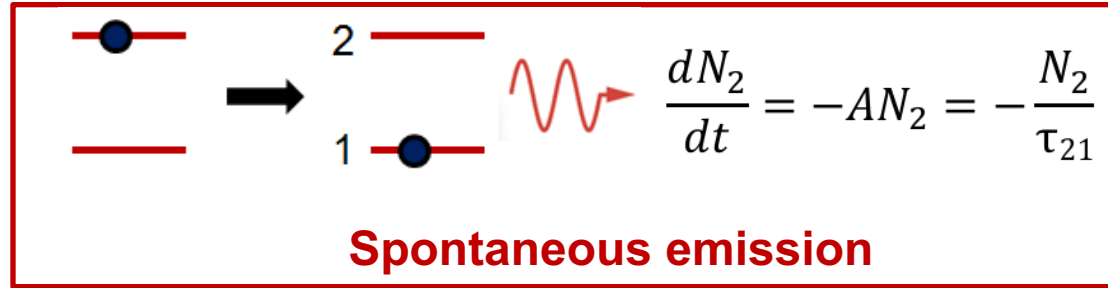
Possible laser cavity configurations

High reflector
($r_1 \approx 100\%$)

Output coupler
(r_2)

High reflector

Output coupler

High reflector

The laser (oscillator) concept explained using a circuit model.

Three phenomena related to light-matter interaction in laser

$$\frac{dN_2}{dt} = -AN_2 = -\frac{N_2}{\tau_{21}}$$

Spontaneous emission

$$\frac{dN_1}{dt} = -BN_1 I$$

Absorption
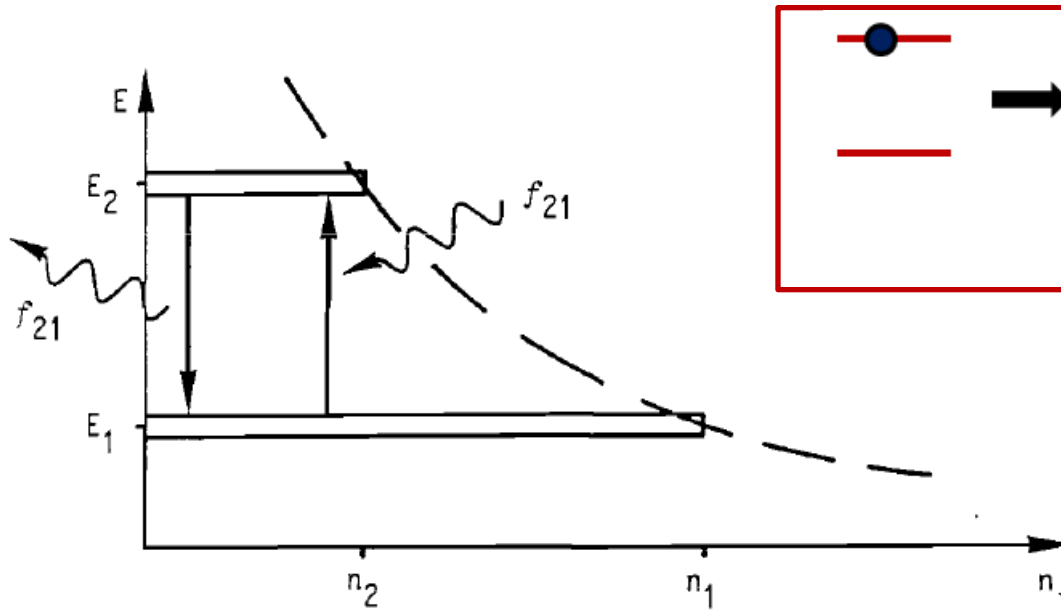
N_1 (N_2) is number of atoms in the lower (higher) energy level.

$$\frac{dN_2}{dt} = -BN_2 I$$

An incident photon triggers an excited atom to transit to a lower state by generating a second photon, which is a "clone" of the incident one—same freq., polarization, and traveling direction etc.

Stimulated emission (Laser: Light Amplification by Stimulated Emission of Radiation)

Population inversion for amplification

Amplification requirement: $N_2 > N_1$

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} \exp\left(\frac{-(E_2 - E_1)}{kT}\right)$$
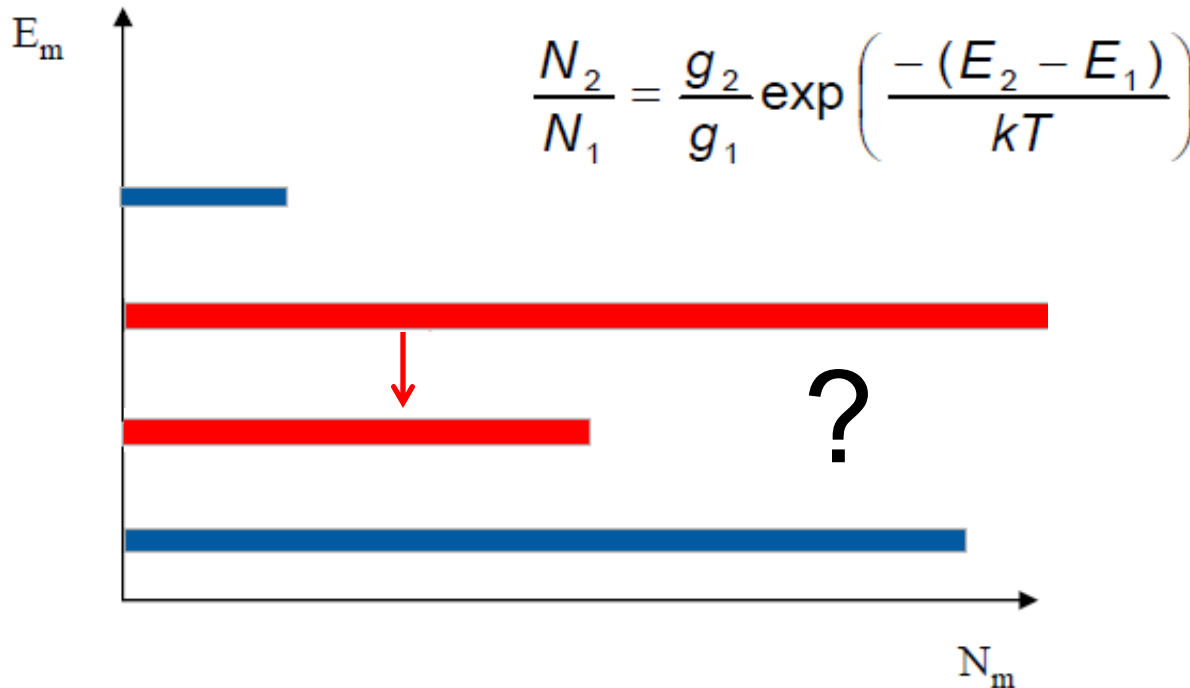
N_i is the number density (also known as the population density) of molecules in state i (i.e., the number of molecules per cm^3).

T is the temperature, and k is Boltzmann's constant = 1.3806503 $\times$ 10^{-23} J/°K

Under thermal equilibrium conditions, the lower energy levels are populated first, and are always more populated than the higher levels.