PC IV: MOLECULAR SPECTROSCOPY /

Molekülspektroskopie

Prof. Oleg Vasyutinskii

Summer Semester: from April 9, 2007 till July 20, 2007

Lectures: Thursday 8:00 – 9:30 (PK11.2)
Friday 11:30 – 12:15 (PK11.2)
Exercises: Friday 12:15 – 13:00 (PK11.2)

URL Internet Skript

Vorlesung: http://www.pci.tu-bs.de/aggericke/PC4

Englisch: http://www.pci.tu-bs.de/aggericke/PC4e_osv/

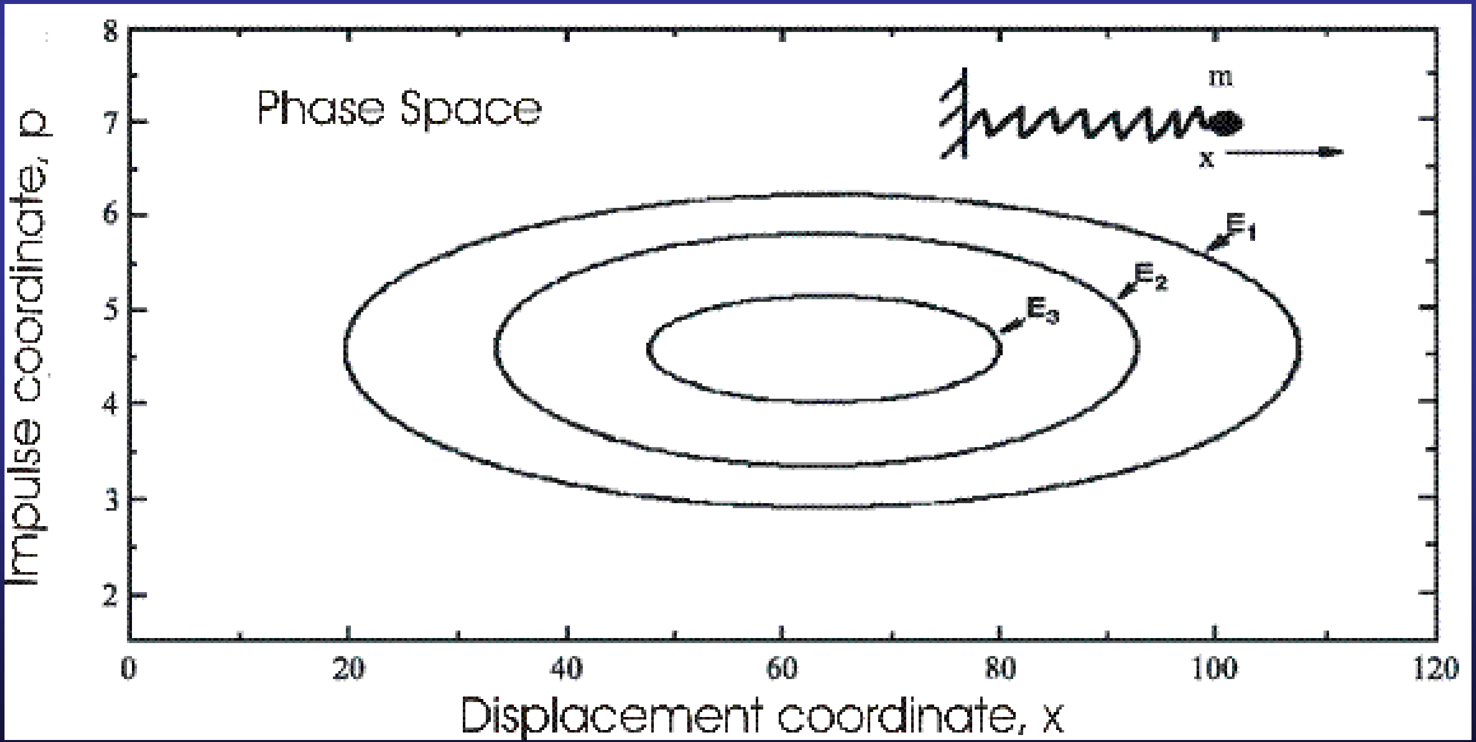
Basis Concepts of Classical Mechanics

The Newton equations of motions describes the movement of particles along well-defined trajectories which are the result of boundary conditions and the forces between them.

For example, let us concider a Harmonic Oscillator (a massive particle on a spring):

$V(x) = \frac{1}{2} kx^2$, $E = p^2/2m + \frac{1}{2} kx^2 \Rightarrow$ $E = \frac{1}{2} m (dx/dt)^2 + \frac{1}{2} kx^2$

Having in mind the energy conservation law, we see that all possible energies are ellipses in the phase space (x ,p): $E = p^2/2m + \frac{1}{2} kx^2$



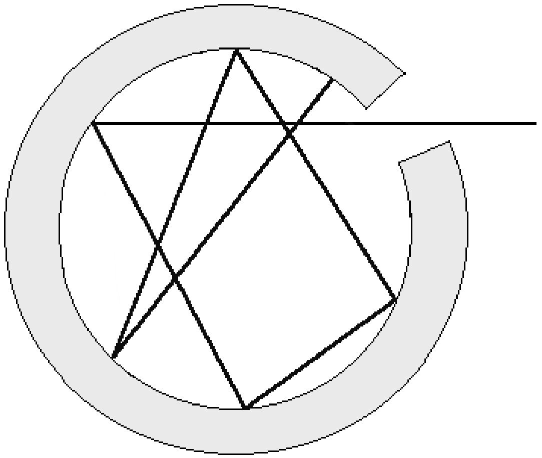
Hamilton Equations

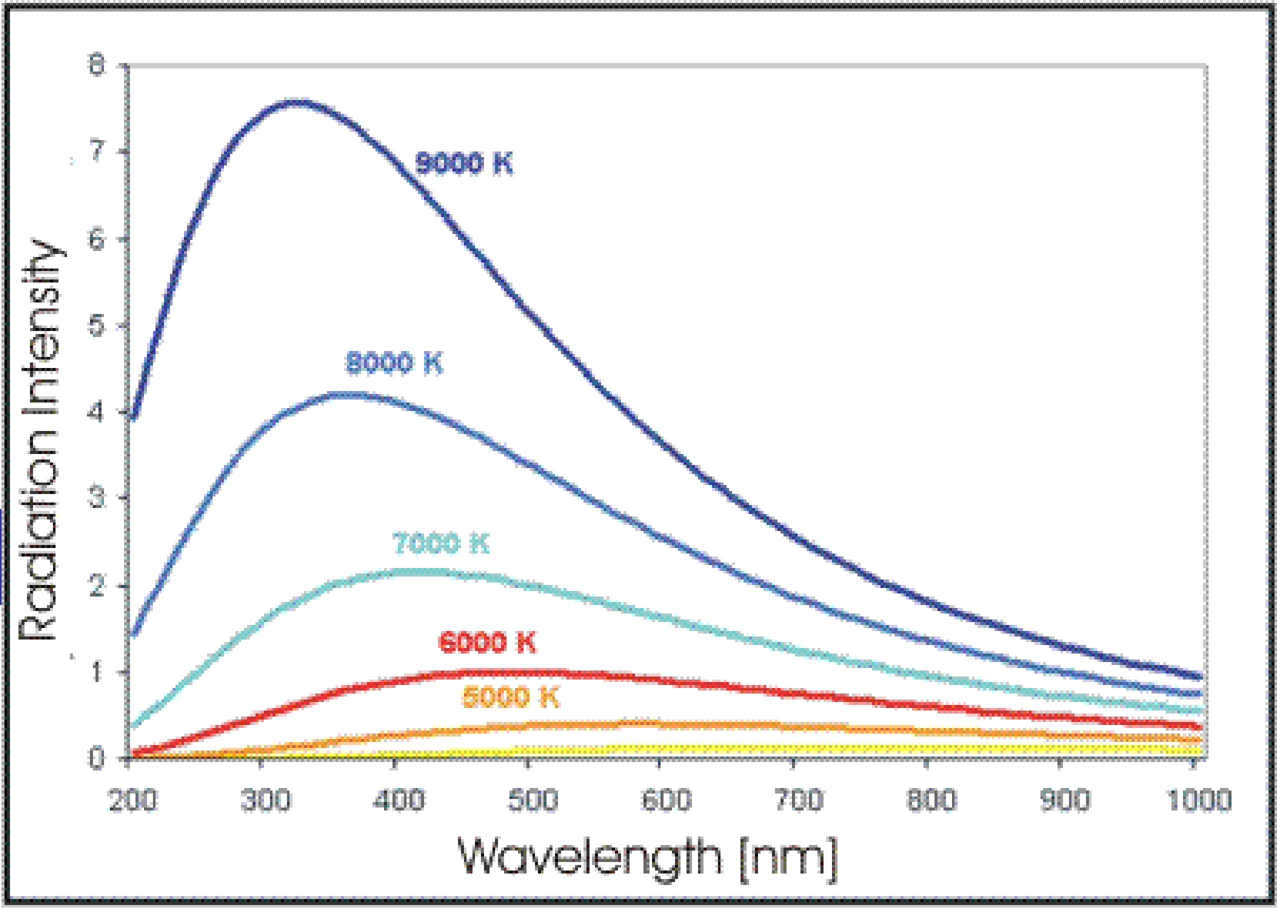
$$dq/_{dt} = {}^{\partial H}/_{\partial p}$$

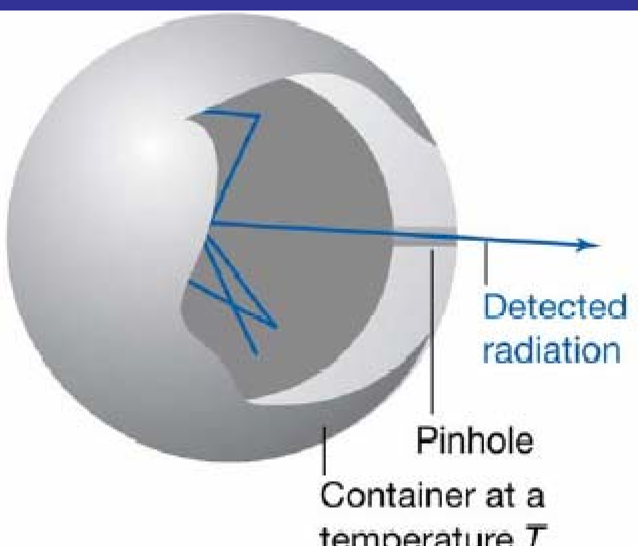
$$dp/_{dt} = - {}^{\partial H}/_{\partial q}$$

* 4. Aug. 1805 in Dublin, Irland
+ 2. Sep. 1865 in Dublin, Irland

Problems of Classical Mechanics: Black Body Radiation.







How can be explained the intensity of black body radiation as function of the radiation wavelength?

Black Body Radiation

In 1900 Max (Karl Ernst Ludwig) Planck first suggested that the radiation energy cannot have all continuum values. He postulated that the energy is always proportional to a certai very small discret portion of energy which cannot be disintegrated. This elementary portion of energy (quant) is proportional to the radiation frequency ν, E = *h* ν , where *h* is the proportionality constant which is now known as Planck constant.

$$h = 6{,}626176 \cdot 10^{-34}\ \mathrm{J{\cdot}s}$$

* 23. April 1858 in Kiel, Schleswig-Holstein

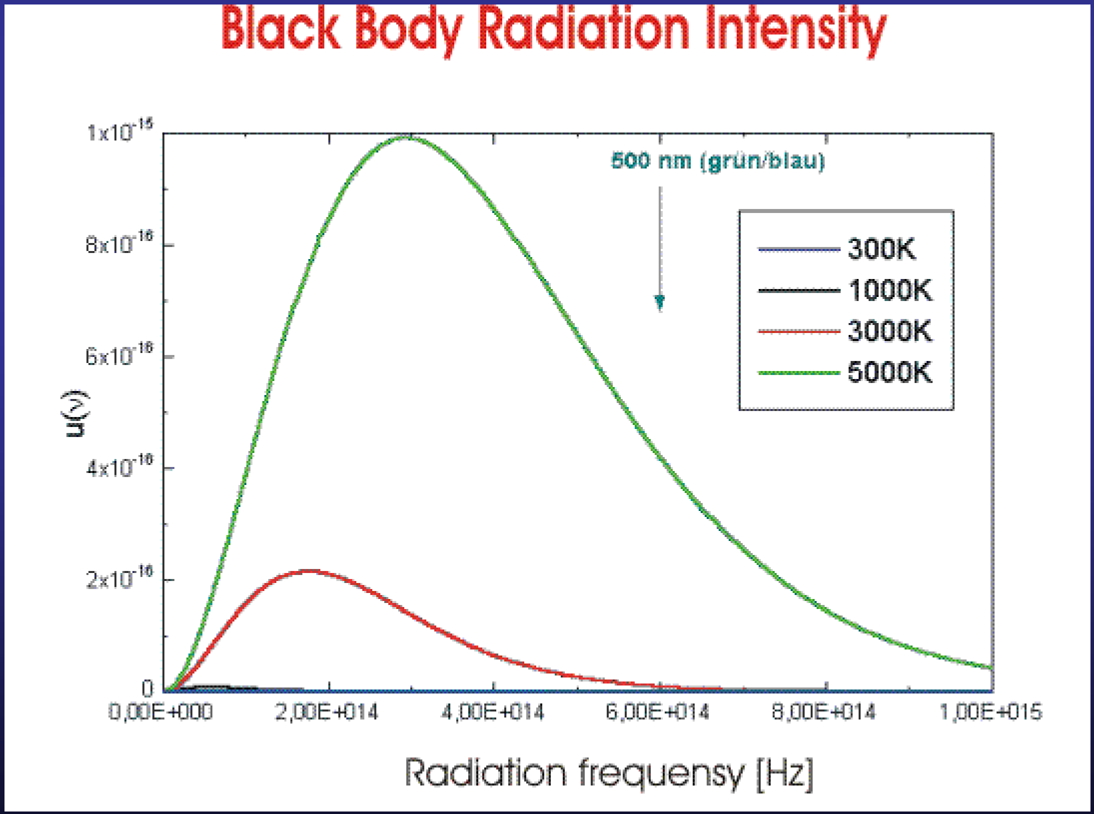
\+ 4. Oktober1947 in Göttingen

Nobelpreis 1918

Planck's Formula

$$u(\nu)d\nu = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/kT}-1}d\nu$$

The Planck's formula was found to be in perfect agreement with experiment. However, the Planck's postulate about existance of the elementary indivisible portion of energy (**quant**) resulted at that time to fierce discussions with the adepts of the classical theory.



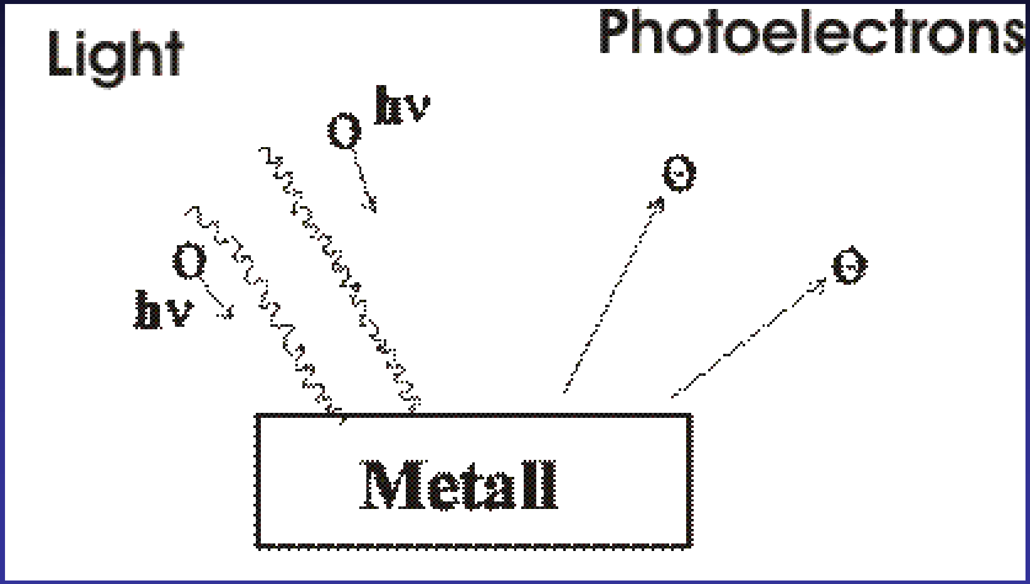
The maximim of the Planck distribution corresponds to the radiation velocity of :

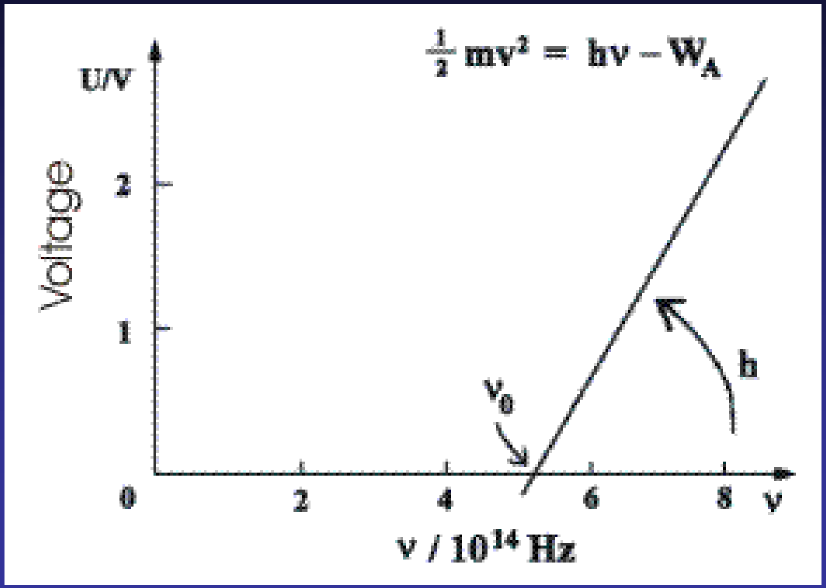
$\nu_{max} = 2{,}8214\ {}^{kT}/_{h}$

which can easily be measured experimentally and thus the Planck constant can be determined. Its value is

$k = 1{,}3806503 \cdot 10^{-23}\ J \cdot K^{-1}$

Problems of Classical Mechanics: Photoeffect





Experiment:

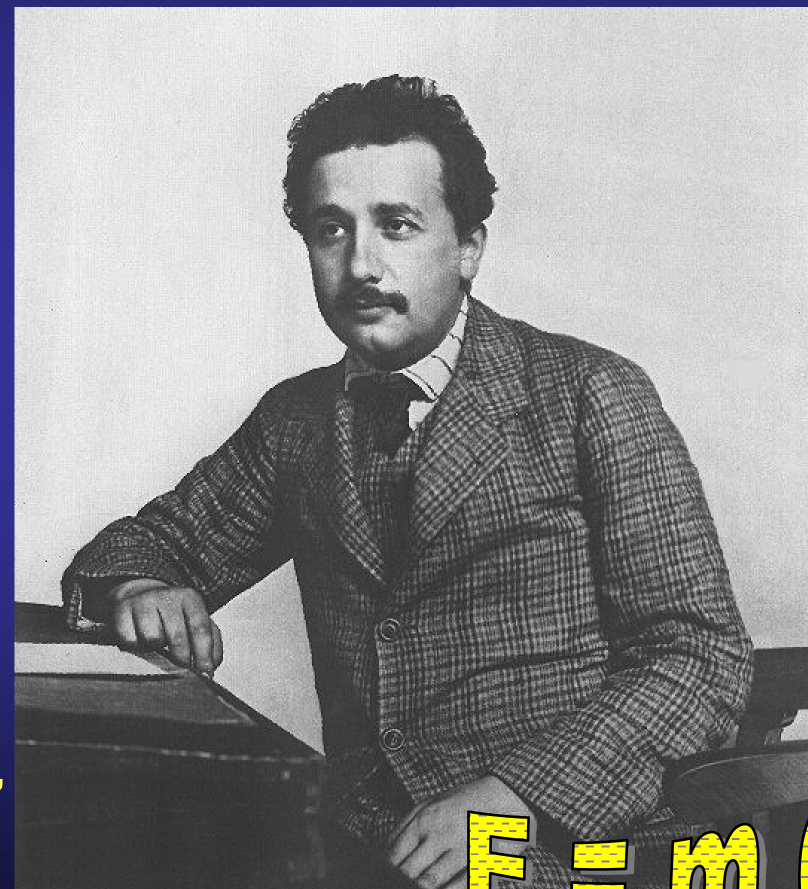
- No photoelectrons are detected under some light frequency for **any** light intensity (the threshold effect).
- The photoelectron energy does not depend on the light intensity.
- The photoelectron energy linearly depends on the light frequency.

Classical Interpretation:
The electromagnetic field of the incident light **E** causes oscillation of the free electrons and pulls them out from the metall. However, this model predicts that the output electron flux is proportional to the light intensity and does not explain the threshold effect and why the electron flux is proportional to the light frequency.

Quantum mechanical interpretation:
The light is absorbed by the metall **quant by quant**. An electron is bound inside the metall and a certain energy (**photoelectric work function**) is needed for extracting it out to the vacuum. The rest of the photon energy is realized as the photoelectron **kinetic energy**. This model perfectly fits all experimental data.

Albert Einstein

*** 14. März 1879 in Ulm, Württemberg**
+ 18. April 1955 in Princeton, New Jersey, USA
Nobel Prize 1921 für Photoeffekt

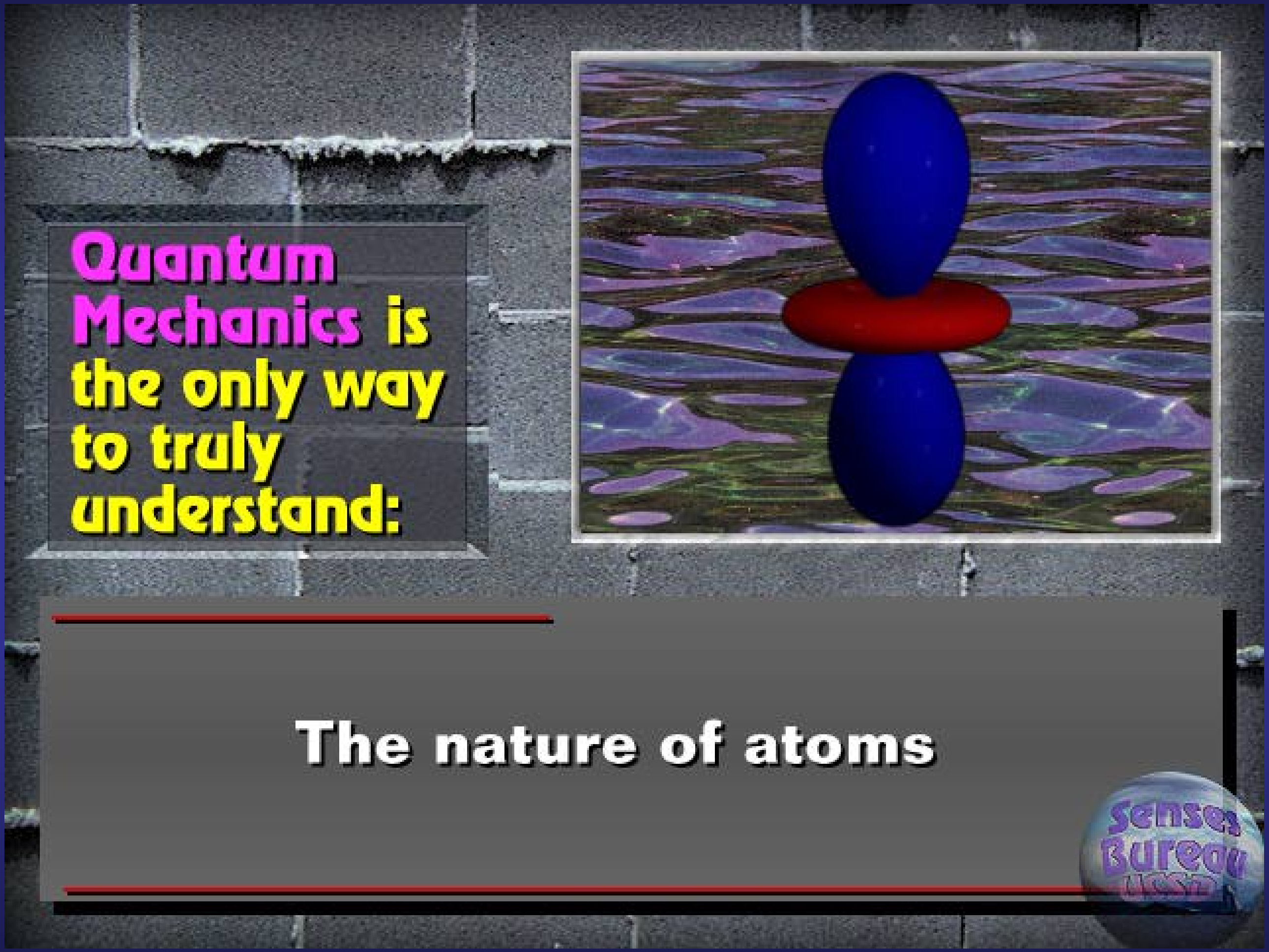


$$E = mc^2$$

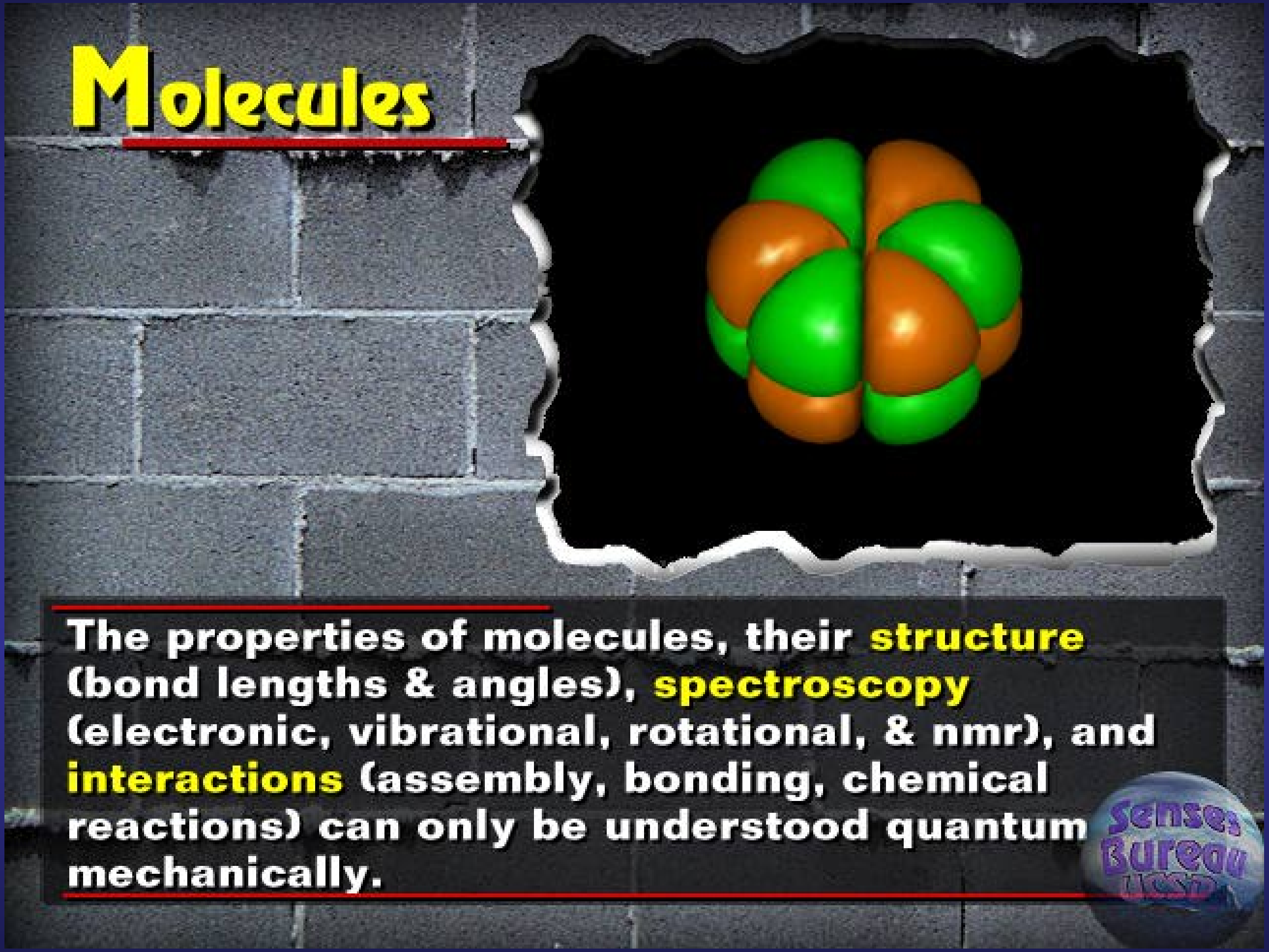
He developed the Theory of Photoeffect, the Theory of Light Absorption my Matter, the Special Relativistic Theory, and the General Ralativistic Theory.

Albert Einstein

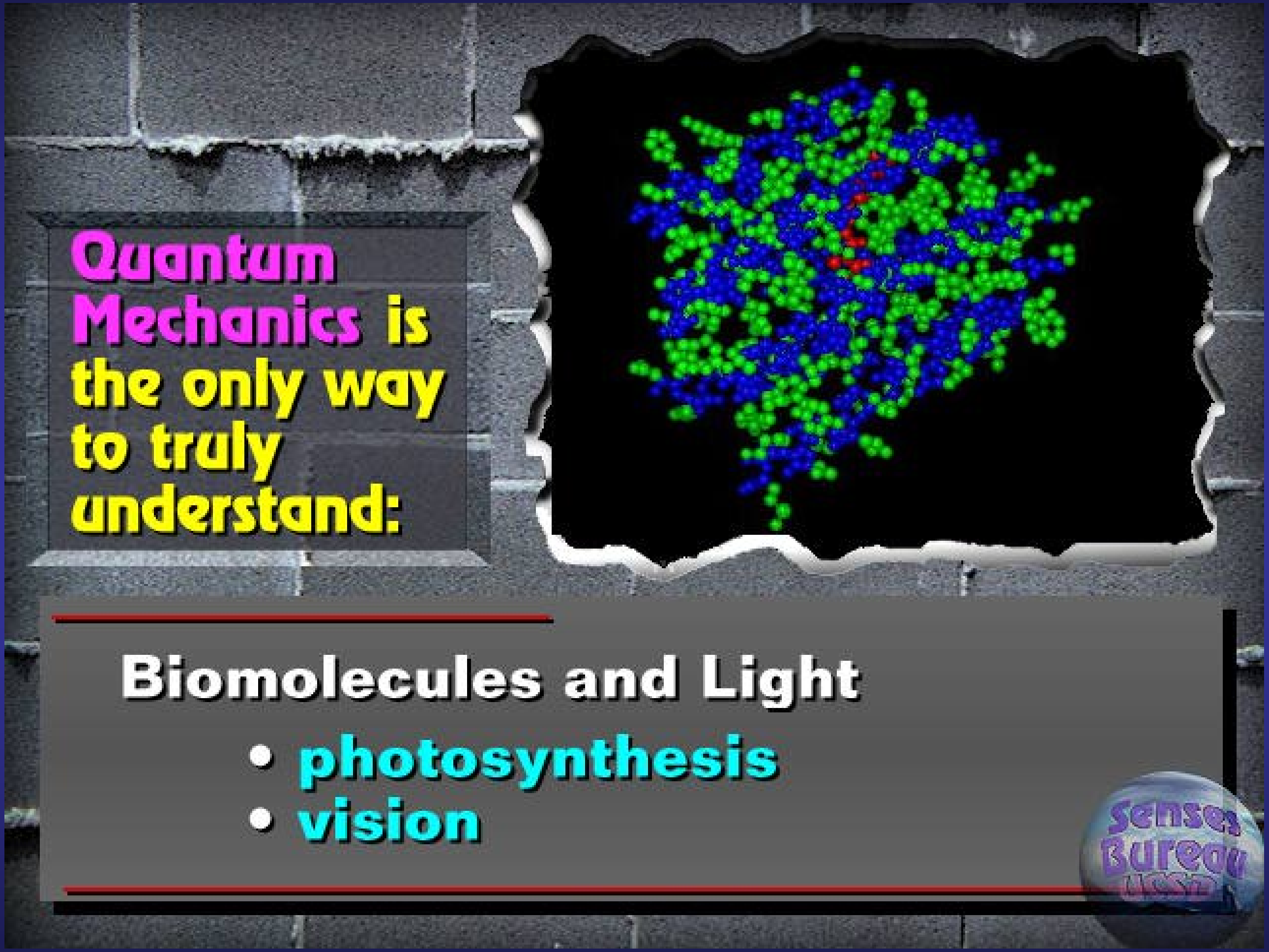
Why Quantum mechanics?



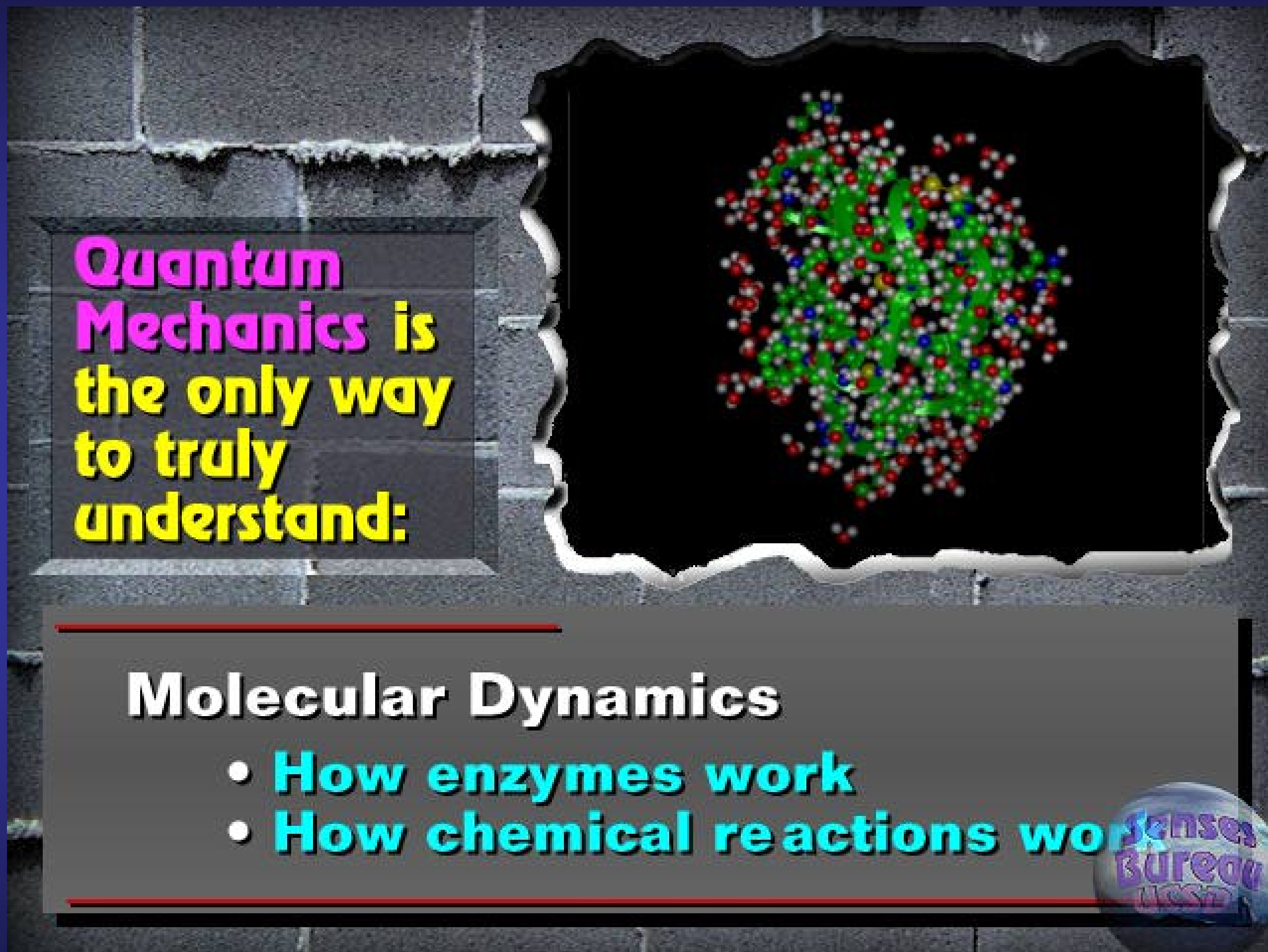
Why Quantum mechanics?



Why Quantum mechanics?



Why Quantum mechanics?



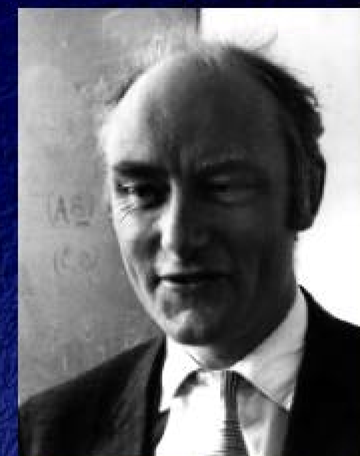
Why Quantum mechanics?

" The underlying physical laws necessary for the mathematical theory of ... the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. "

P.A.M. Dirac
1929

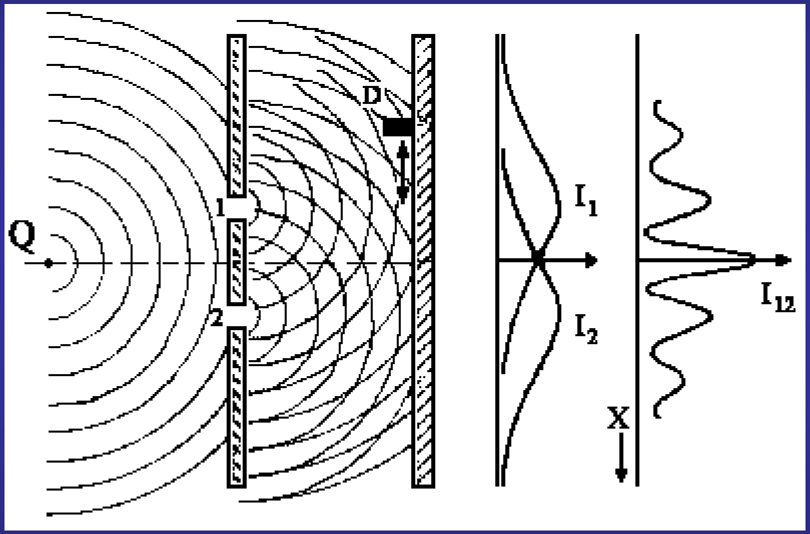
Why Quantum Mechanics?

" The ultimate aim of the modern movement in biology is in fact to explain all biology in terms of physics and chemistry... Quantum mechanics, together with our empirical knowledge of chemistry, appears to provide us with a 'foundation of certainty' on which to build biology."



Francis Crick
1966

Interference of Electromagnetic Waves



$\phi = A\, e^{-i\omega t + ikx}$

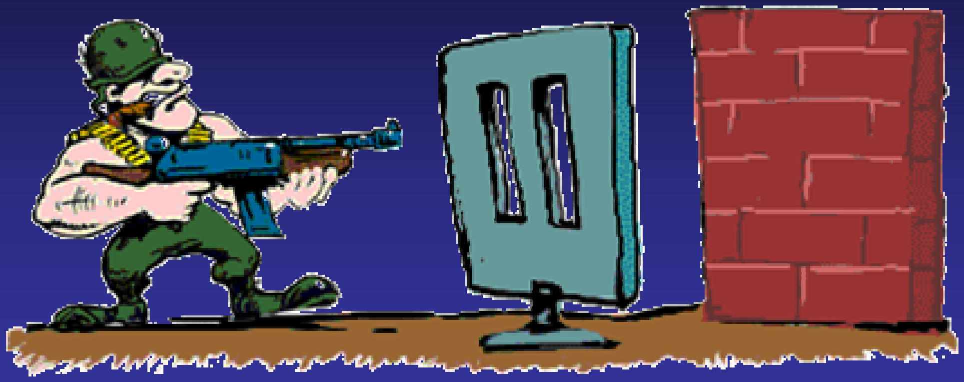
$\omega = 2\pi\nu$: Wave Frequency

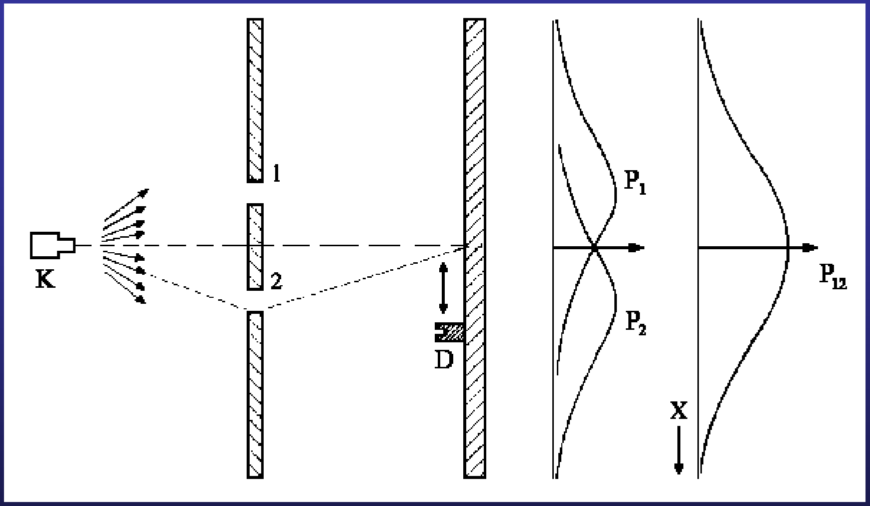
$\lambda = c / \nu$: Wavelength

$\mathbf{k} = {}^{2\pi}/_{\lambda}$: Wavevector

Total Wave Intensity: $I = |\phi|^2$

Experimente with particles





$$P_{12} = P_1 + P_2$$

de Broglie: a Particle is a Wave

De Broglie's Dissertation “Recherches sur la théorie des quanta“ in 1924 at the firts time gave a relationship between a particle mass m, its velocity v, and the corresponding wavelength λ:

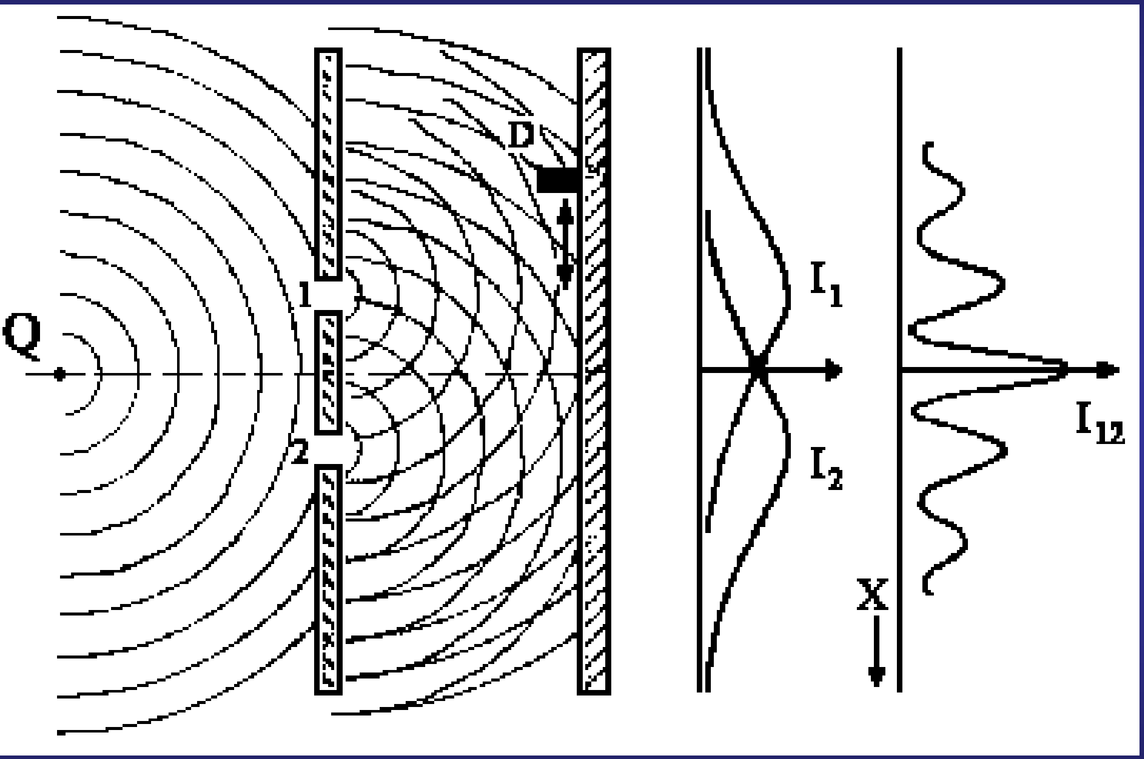
Wavelength: $\lambda = {}^{h}/_{mv}$

Louis Victor Pierre Raymond duc de Broglie
*** 15. Aug. 1892 in Dieppe, France**
+ 19. März 1987 in Paris, France

Nobelpreis 1929

Interference of Matter Waves

$$\phi = A\, e^{-i\omega t + ikx}$$



$\omega = 2\pi\, {}^{E}/_{h}$: Frequency

$\mathbf{k} = {}^{2\pi}/_{\lambda} = {}^{p}/_{\hbar}$: Wavevector

Probability to Detect the Particle

$$I = |\phi|^2$$

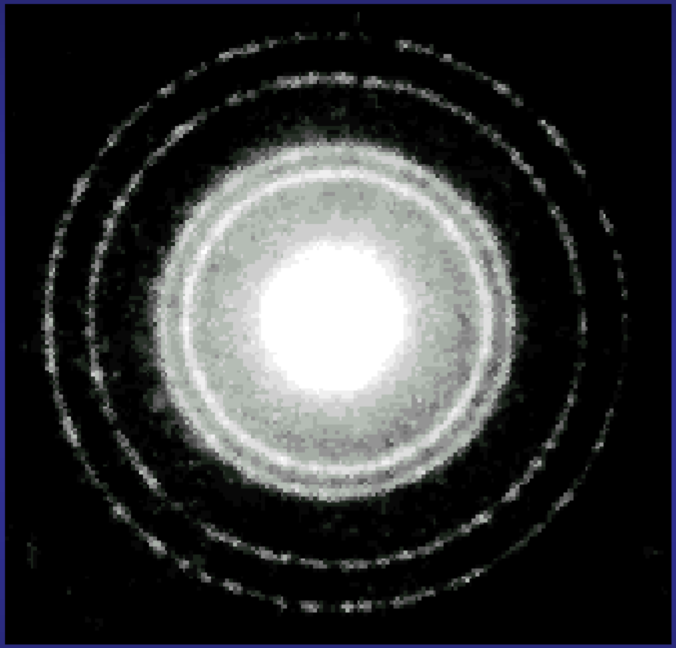
$$\phi = \phi_1 + \phi_2$$

$$\mathbf{I = |\phi_1 + \phi_2|^2}$$

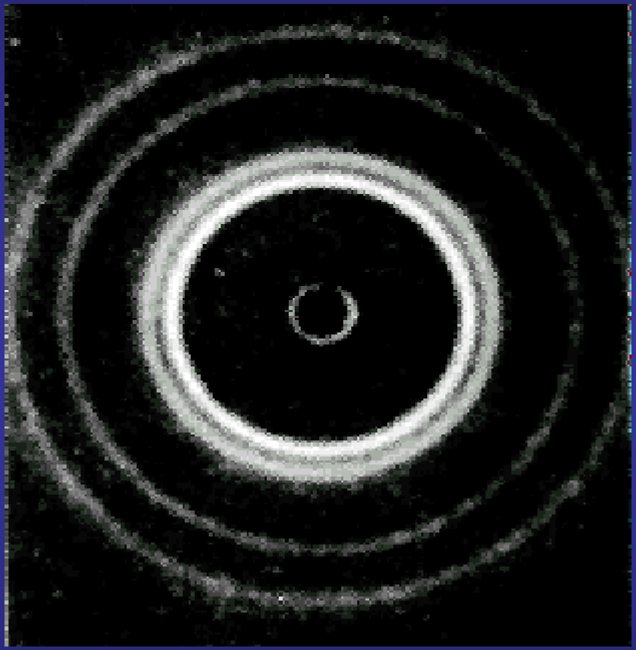
$$I = I_1 + I_2 + 2(I_1 I_2)^{1/2} \cdot \cos \Delta\varphi$$

Where $\Delta\varphi$ is the phase difference

Experiment: a Particle is a Wave

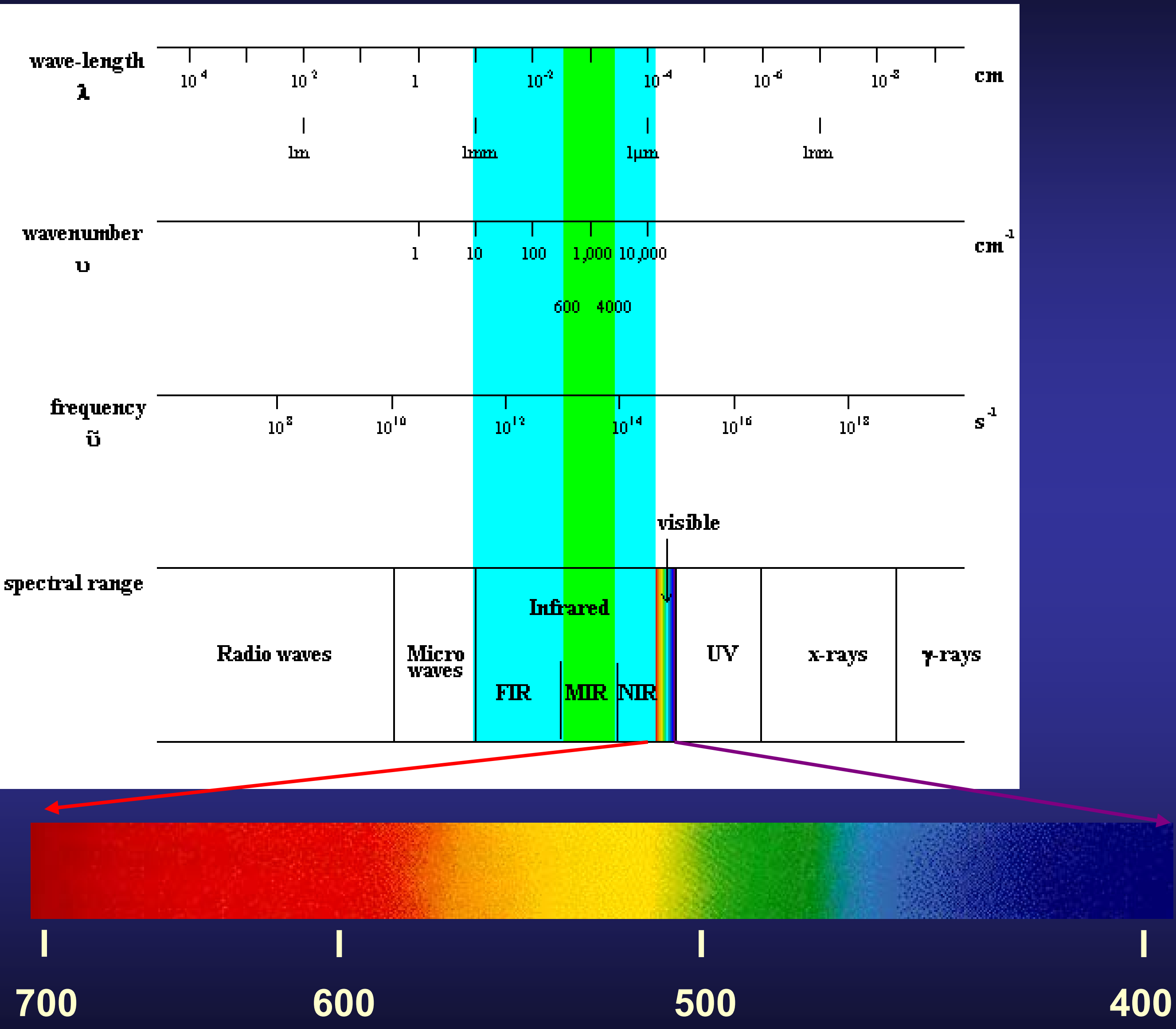


Diffraction of Elecrtons



Diffraction of X-Rays

Spectrum of Electromagnetic Waves



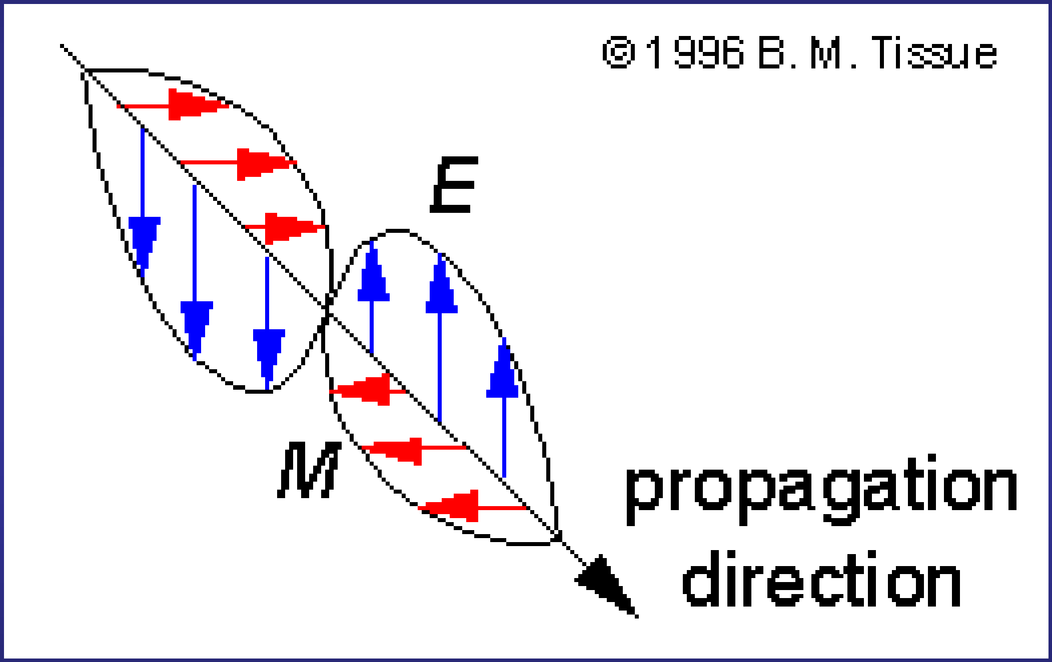
Spectral Areas

Visible Light

Electromagnetic Spectrum

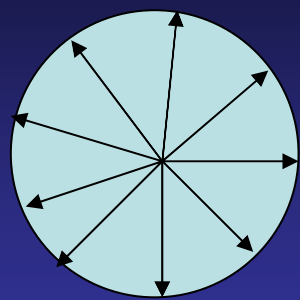
Type of Radiation	Frequency Range (Hz)	Wavelength Range	Type of Transition
gamma-rays	10^{20}-10^{24}	<1 pm	nuclear
X-rays	10^{17}-10^{20}	1 nm-1 pm	inner electron
ultraviolet	10^{15}-10^{17}	400 nm-1 nm	outer electron
visible	4-7.5x10^{14}	750 nm-400 nm	outer electron
near-infrared	1x10^{14}-4x10^{14}	2.5 μm-750 nm	outer electron molecular vibrations
infrared	10^{13}-10^{14}	25 μm-2.5 μm	molecular vibrations
microwaves	3x10^{11}-10^{13}	1 mm-25 μm	molecular rotations, electron spin flips*
radio waves	<3x10^{11}	>1 mm	nuclear spin flips*

Electromagnetic Radiation



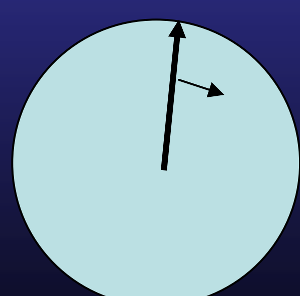
Light Polarization

E



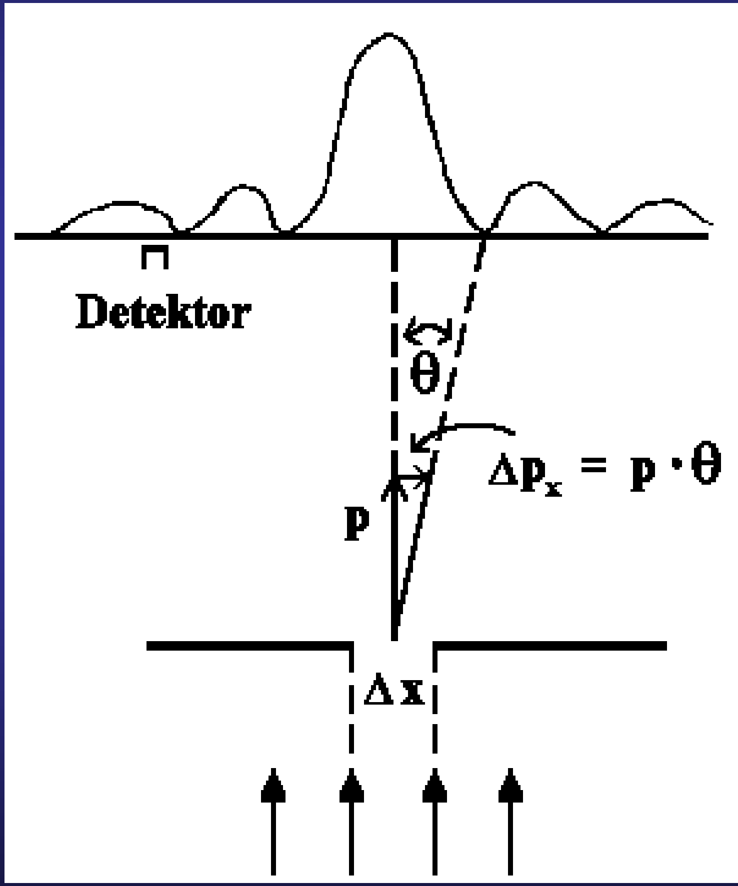
Unpolarized light

Linearly polarized light



Circularly polarized light

Diffraction on a Slit: The Uncertainty Principle



Interference: $\theta = {}^{\lambda}/_{(2\,\Delta x)}$

Impulse: $\Delta p_x \approx p \bullet \theta = p\,{}^{\lambda}/_{(2\,\Delta x)}$

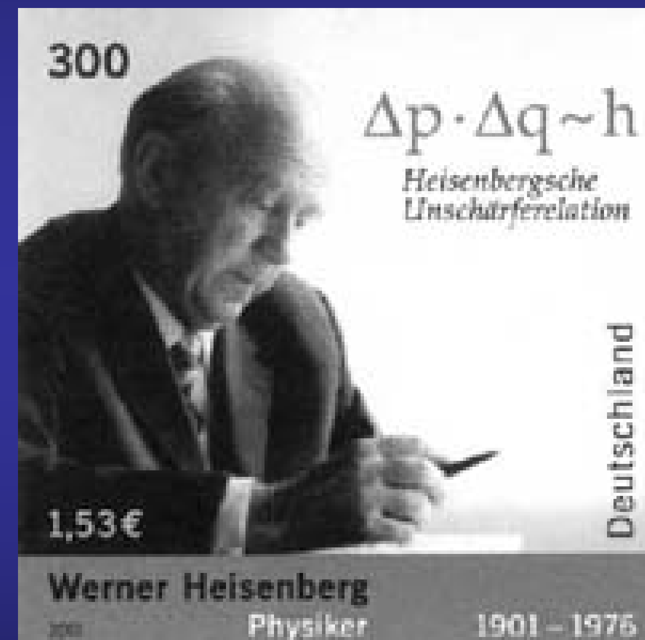
De Broglie wavelength: $\mathbf{p} = {}^{\mathbf{h}}/_{\lambda}$

$$\Delta x \cdot \Delta p_x \approx \hbar$$

Planck-Constante $\hbar = h/2\pi$

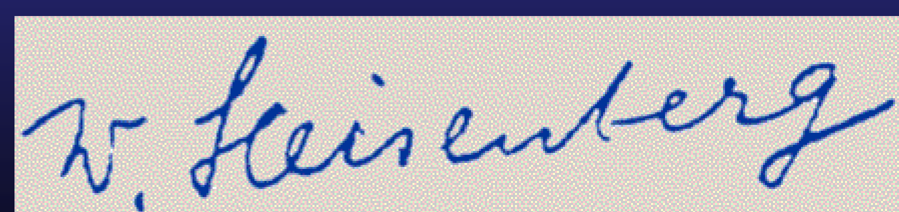
$h = 6{,}6260755 \cdot 10^{-34}$ J·s

Werner Karl Heisenberg

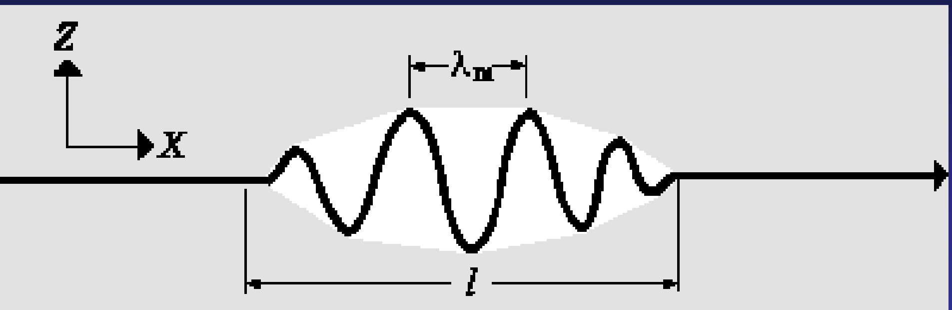


1927 Unschärferelation

* 5. Dez. 1901 in Würzburg
+1. Feb. 1976 in München
Nobelpreis 1932

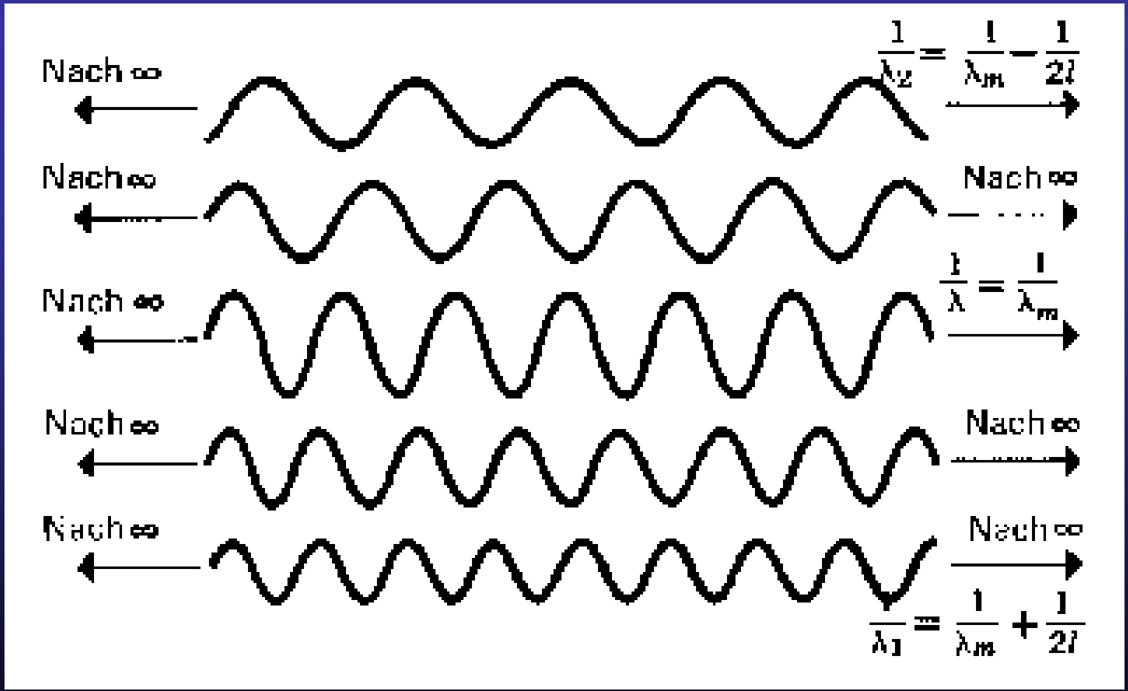


A Particle as a Wavepacket

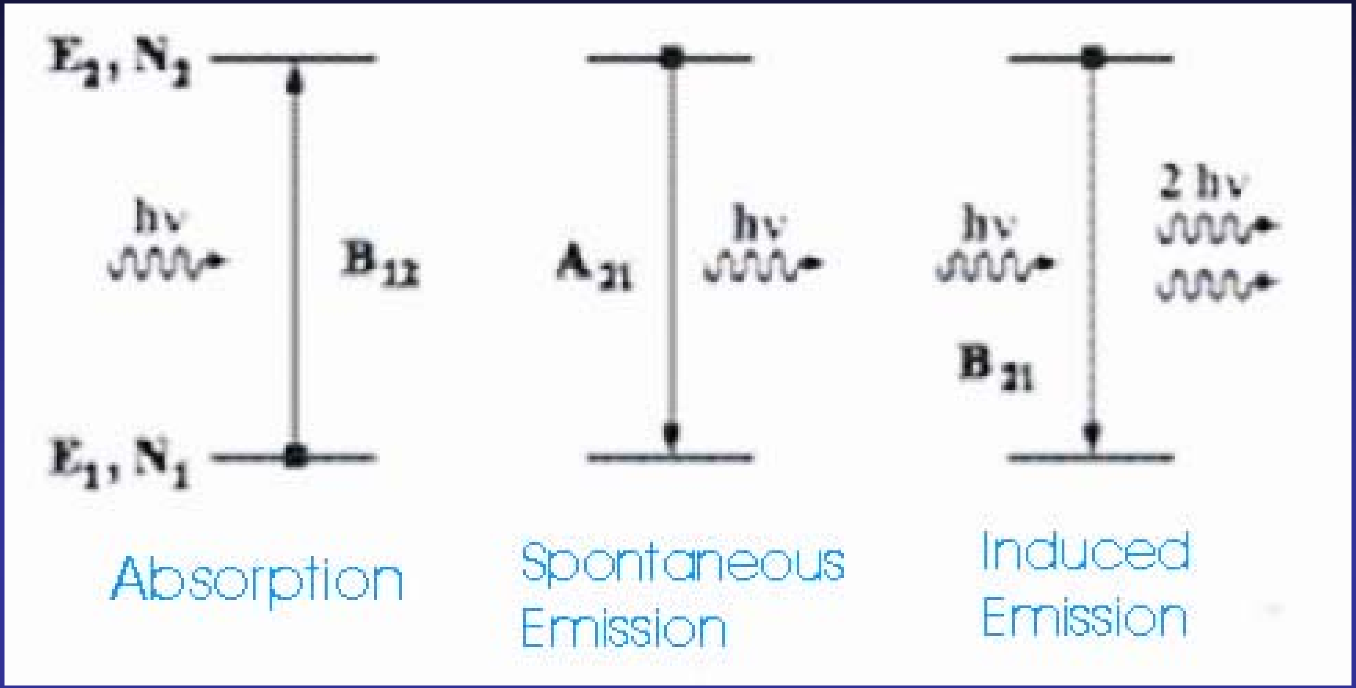


The wavepacket can be presented as a superposition of many harmonic waves with different wavelengths (impulses).

$$\Phi(x) = \int_{-\infty}^{\infty} w(p)\, e^{i\frac{p}{\hbar}x}\, dp, \qquad p = \frac{2\pi\hbar}{\lambda}$$



Einstein: Interaction of Light with Radiation



$^{dN_2}/_{dt} = B_{12} \cdot u(\nu) \cdot N_1$ $\quad$ $^{dN_2}/_{dt} = -A_{21} N_2$ $\quad$ $^{dN_2}/_{dt} = -B_{21} \cdot u(\nu) \cdot N_2$

$\mathbf{B_{21} / B_{12} = g_2 / g_1}$ $\quad$ $\mathbf{A_{21} / B_{12}} = 8\pi h \, \nu^3 / c^3$

Three Main Principles of Quantum Mechanics

1. The probability of an experimental event **P** is given by the square of a complex number Φ which is called the **probability amplitude, or the wave function**:

$$P = |\Phi|^2 = \Phi \cdot \Phi^*$$

2. If the event can be realized through indistinguishable ways each described by the probability amplitudes Φ_1 , Φ_2 , ets., the total probability amplitude Φ can be found as a linear superposition of the amplitudes Φ_1 and Φ_2 (Superposition Principle):

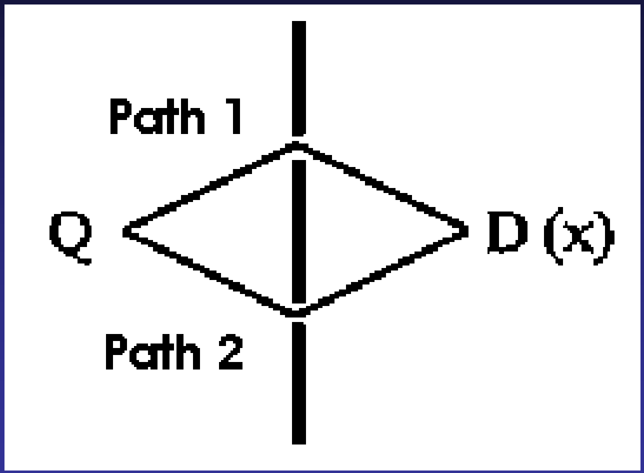
$$\Phi = a_1\Phi_1 + a_2\Phi_2$$

$$P = |\Phi|^2 = |a_1\Phi_1 + a_2\Phi_2|^2 \quad \leftarrow \text{Interference}$$

3. If the experiment allows to determine which alternative is realized, the total probability of the event **P** is the sum of probabilities P_1 and P_2 .

$$P = P_1 + P_2 = |a_1\, \Phi_1|^2 + |a_1\, \Phi_2|^2 \quad \leftarrow \text{no Interference}$$

<bra| und |ket> Vectors



< to | from >

The total probability amplitude:

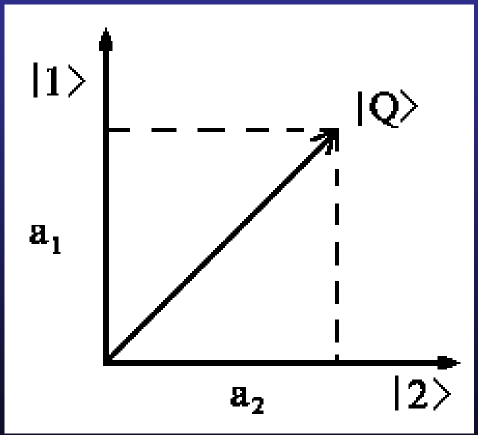
$$\langle x|Q\rangle = \Sigma_{i=1} \langle x|i\rangle\langle i|Q\rangle$$

$$\Sigma_{i=1} |i\rangle\langle i| = 1$$

The values $\langle i|Q\rangle = a_i$ show the contributions from the slits 1 and 2 to the total amplitude:

$$\langle x|Q\rangle = a_1\langle x|1\rangle + a_2 \langle x|2\rangle \qquad \psi(x) = a_1\phi_1(x) + a_2\phi_2(x)$$

$$|Q\rangle = a_1 |1\rangle + a_2 |2\rangle$$



Paul Adrien Maurice Dirac

* 8. Aug. 1902 in Bristol, England
+ 20. Okt. 1984 in Tallahassee, Florida, USA

Nobelpreis 1933

Comparison of the Vector and Amplitude Notations

$|Q\rangle = a_1\,|1\rangle + a_2\,|2\rangle + \ldots$

$\psi(x) = a_1\phi_1(x) + a_2\phi_2(x) + \ldots$

$P_i = |a_i|^2$

$P_i = |a_i|^2$

$\Sigma_x \langle i|x\rangle \langle x|i\rangle = \mathbf{1}$ and $\Sigma_x |x\rangle\langle x| = \mathbf{1}$

$\langle i|i\rangle = 1$ normalization

$\int_{-\infty}^{\infty} |\phi_i(x)|^2 dx = \mathbf{1}$

$\langle i|k\rangle = 0 \quad (i \neq k)$ orthogonality

$\int_{-\infty}^{\infty} \phi_i(x)^* \phi_k(x)\, dx = \mathbf{0} \quad (i \neq k)$

$\Sigma_i P_i = 1$

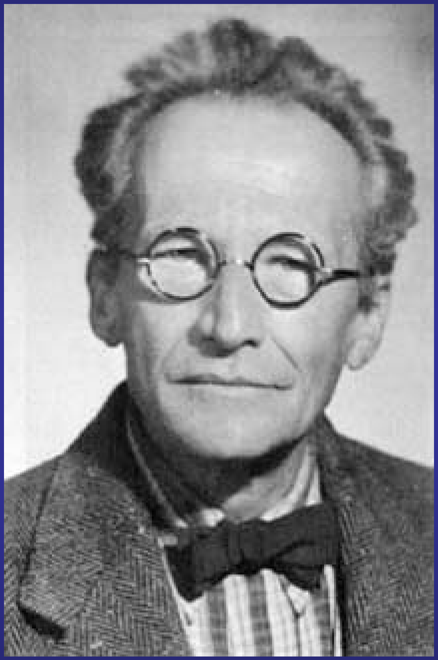
$\Sigma_i |a_i|^2 = 1$

Calculation of the Probability Amplitude (Wavefunction)

There are three mathematically equivalent ways of calculation of the probability amplitude.

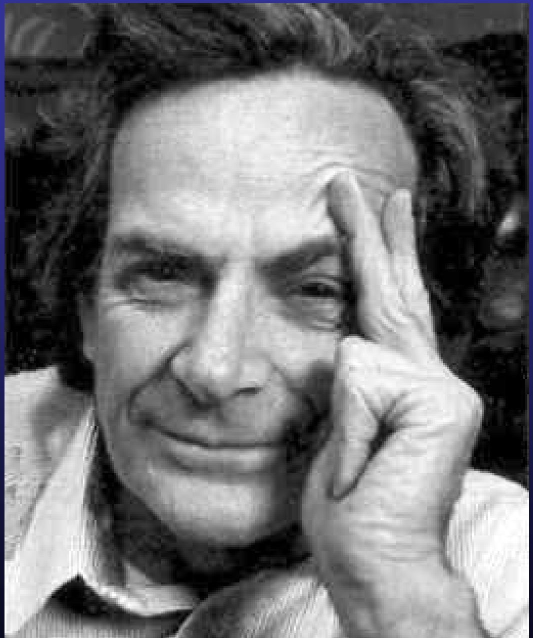
1) Matrix algebra
Werner Heisenberg
Nobelpreis 1932

* 5. Dez. 1901
\+ 1. Feb. 1976



2) Differential equation, DGL
Erwin Schrödinger
Nobelpreis 1933

* 12. Aug. 1887 in Erdberg, Wien
\+ 4. Jan. 1961 in Wien



3) Tragectory integrals
Richard Feynman; Nobelpreis 1965

* 11. Mai 1918 in Far Rockaway, New York
\+ 15. Feb. 1988 in Los Angeles

The Schrödinger Equation

Time-independent Schrödinger Equation:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right] \psi(\mathbf{x}) = E\,\psi(\mathbf{x}) \qquad \text{(1 dimension)}$$

$$\left[-\frac{\hbar^2}{2m}\Delta + V(x,y,z)\right] \psi(\mathbf{x,y,z}) = E\,\psi(\mathbf{x,y,z}) \qquad \text{(3 dimensions)}$$

Where Δ is the Laplace operator: $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Time-dependent Schrödinger Equation:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right] \psi(\mathbf{x,t}) = i\hbar\,\frac{\partial}{\partial t}\,\psi(\mathbf{x,t})$$

Normalization

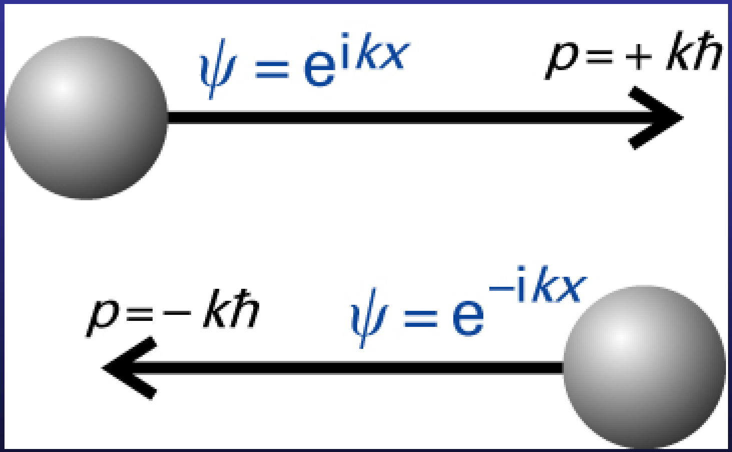
$$\int_{-\infty}^{+\infty} |\psi(x,y,z)|^2 \, dx\, dy\, dz = 1$$

Schrödinger Equation for a Free Particle

If $V(x) = 0 \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(\mathbf{x}) = E\,\psi(\mathbf{x})$

The solution (plane wave) is:

$\Psi(\mathbf{x}) = A\,e^{ikx} + B\,e^{-ikx}$ where $k^2 = 2Em/\hbar^2$

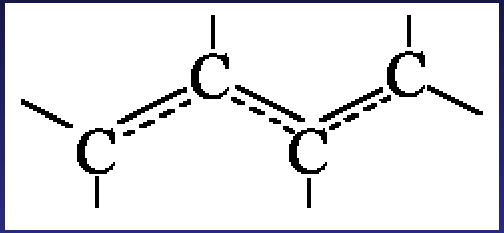


A Particle in a One-Dimensional Box

The Schrödinger Equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n\psi_n(x)$$

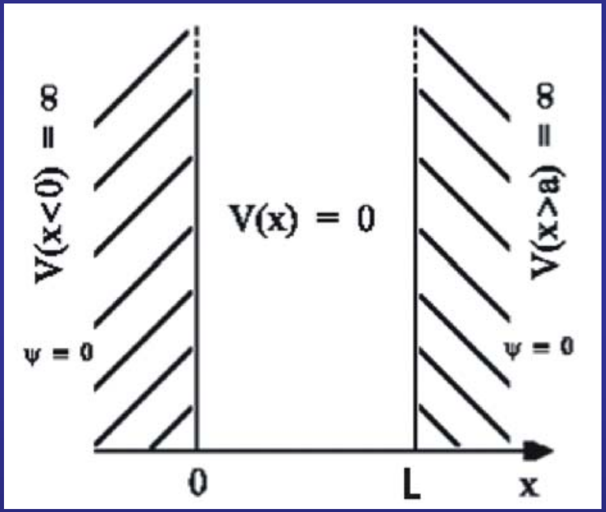
A Particle in a One-Dimensional Box



In conjugated dye molecules the π-electrons behave like a free particles moving along the molecular chain.

The Schrödinger equation:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$



With boundary conditions: $\psi(0)=0$ und $\psi(L)=0$.

The solution is:

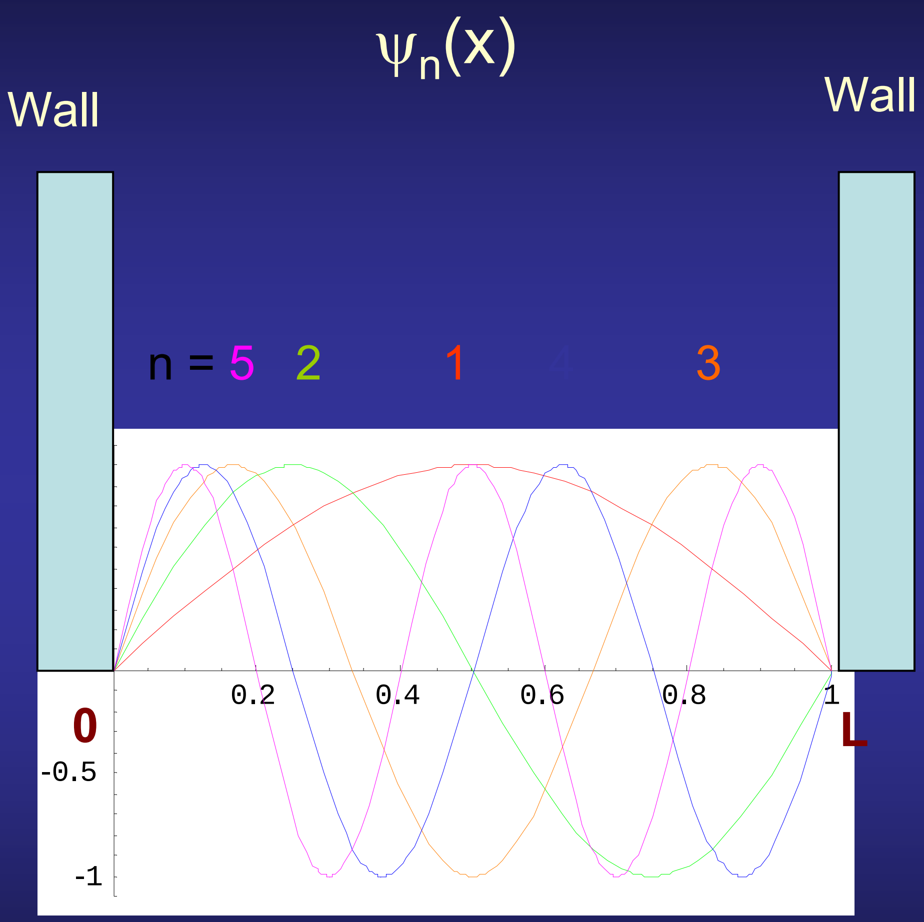
$$E_n = \frac{h^2}{8mL^2} n^2 \qquad \text{where} \quad n = 1, 2, 3, \ldots$$

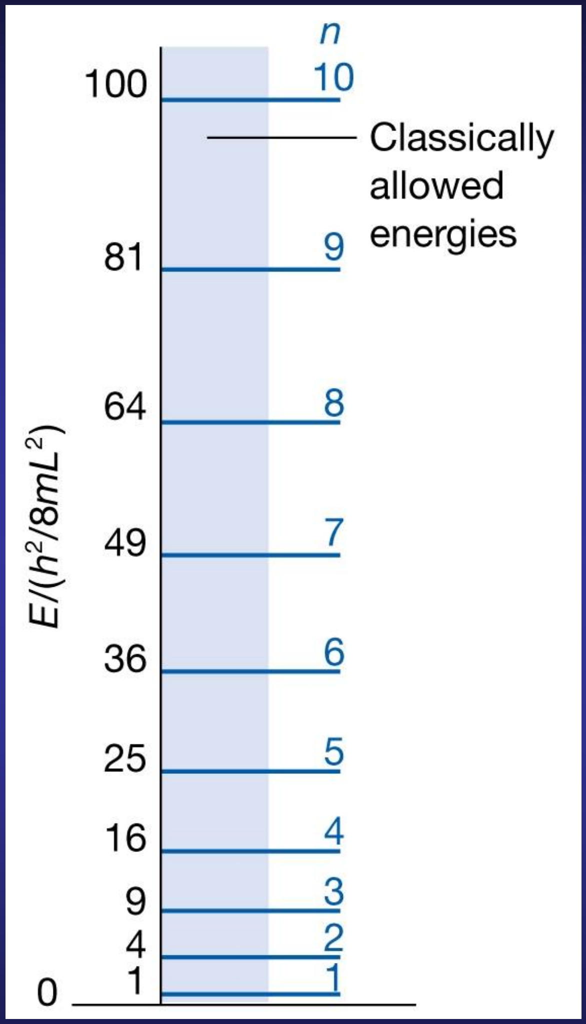
$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(n\pi \frac{x}{L}\right)$$

The factor $\left(\frac{2}{L}\right)^{1/2}$ results from the wavefunction normalization:

$$\int_0^L |\psi_n|^2 dx = \int_0^L C^2 \sin^2\left(n\pi \frac{x}{L}\right) dx = C^2 \cdot \tfrac{1}{2} L = 1$$

A Particle in a One-Dimensional Box

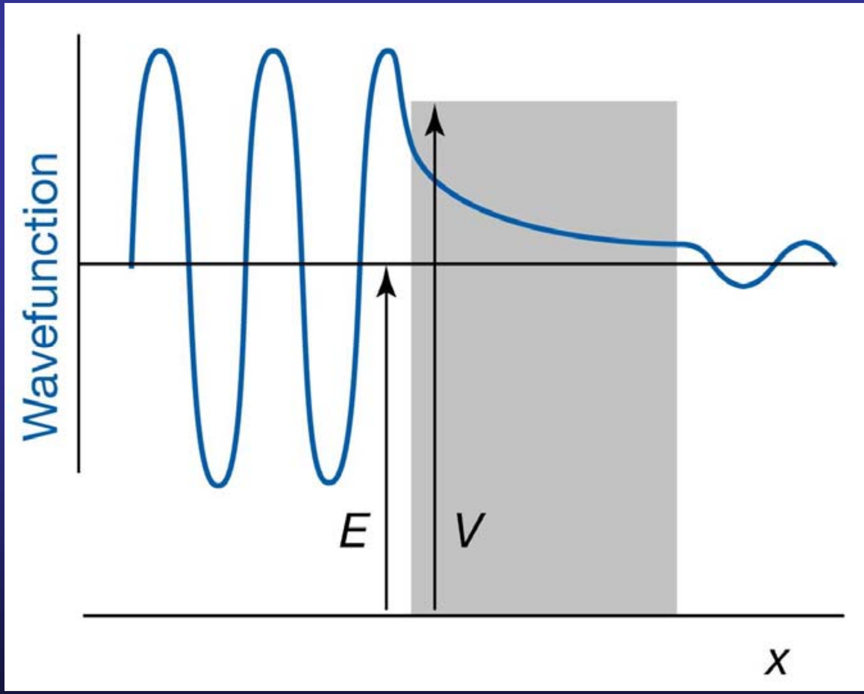


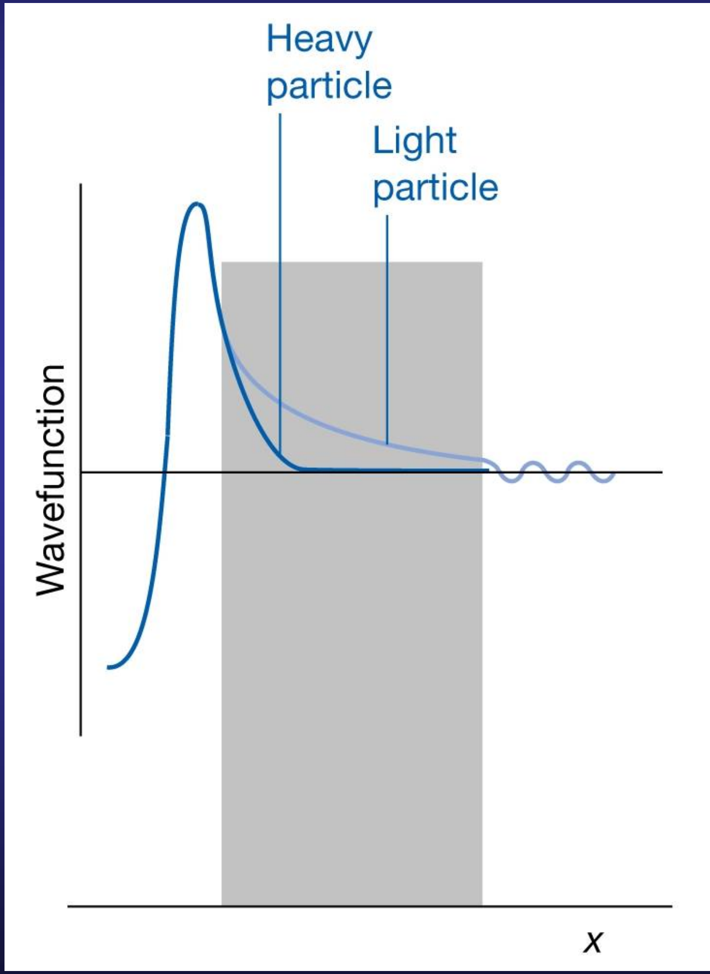


$\psi_n(x) = (2/L)^{1/2} \sin(\pi n x/L)$

$E = n^2h^2/8mL^2$

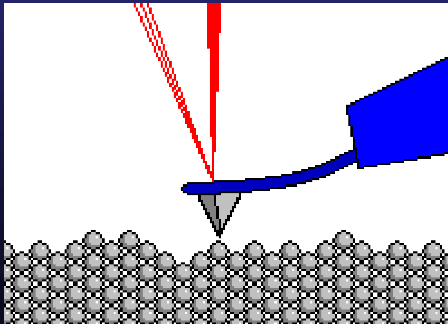
What Happens if a Wall is Not Infinitely High? Tunneling





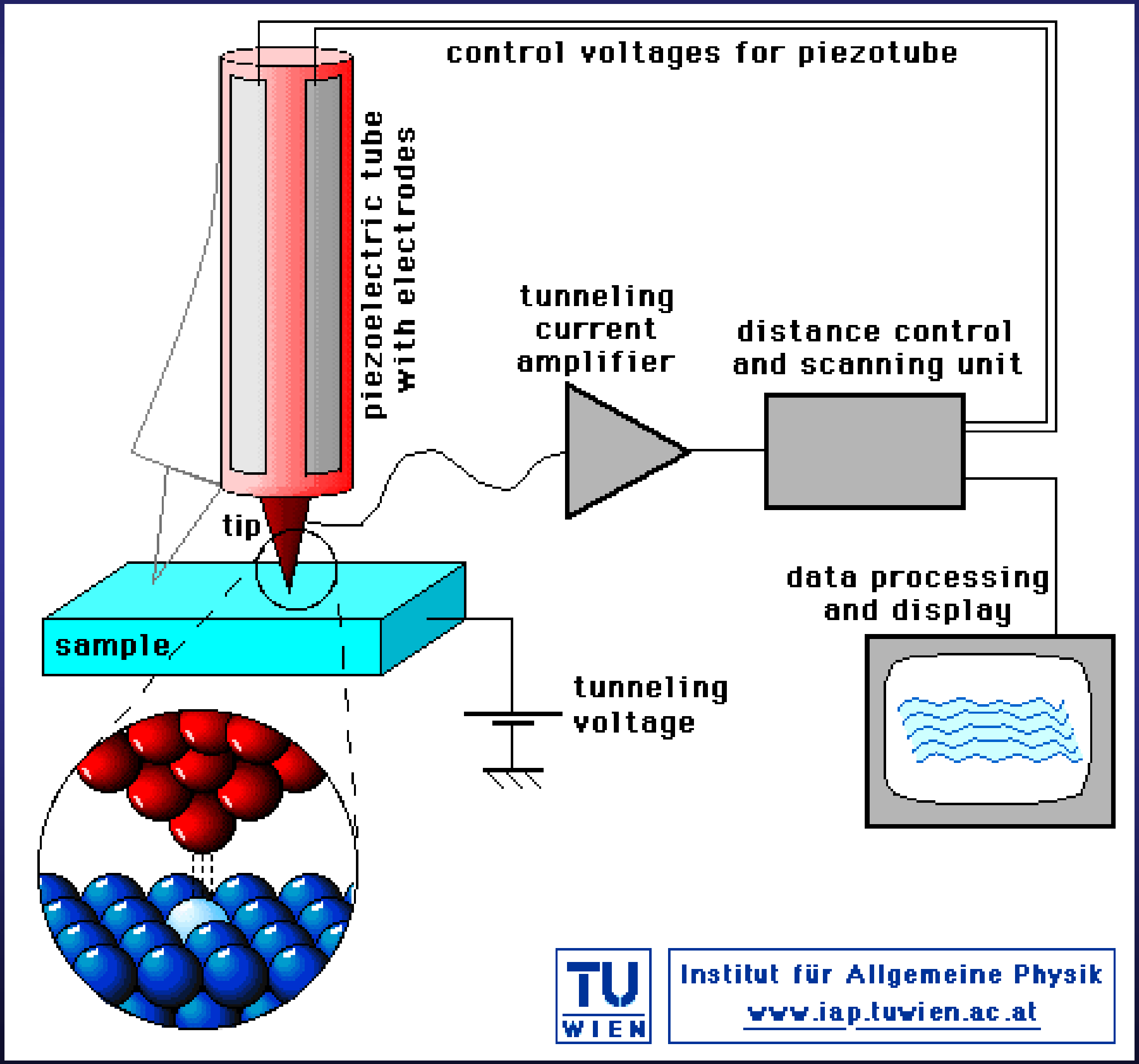
Tunneling

Tunneling Microscope

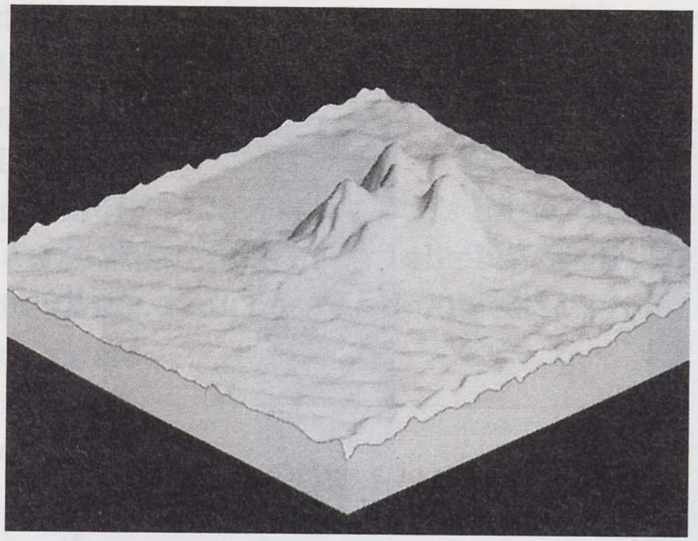


Example: Scanning Tunneling Microscope

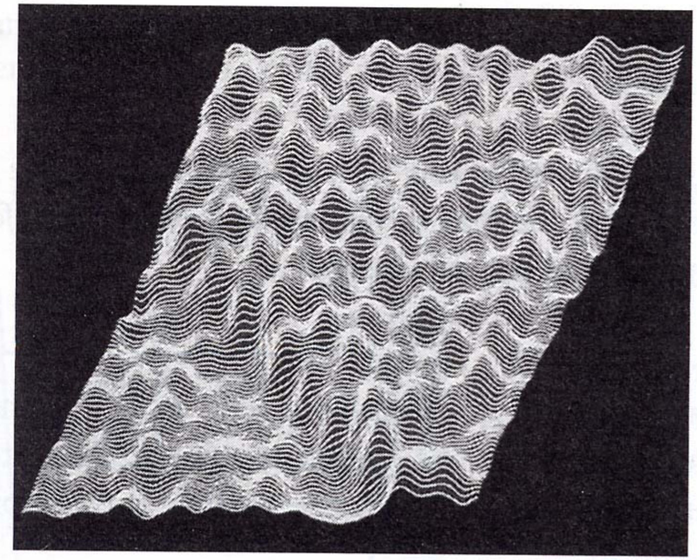
Nobel Prize 1986
Gerd Binning and Heihrich Rohrer



Scanning Tunneling Microscope

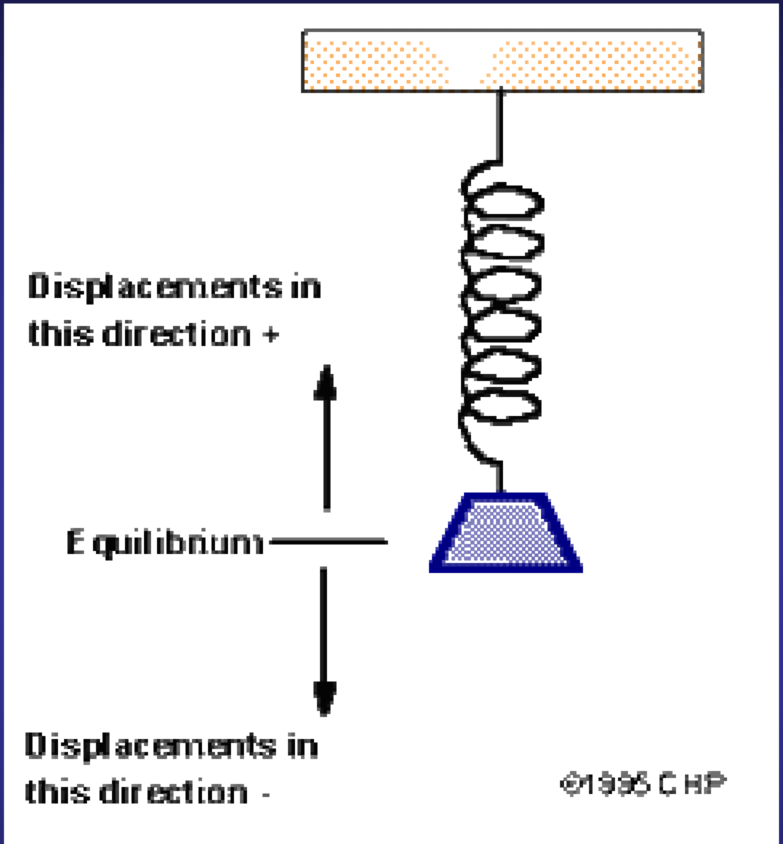


A scanning tunnelling microscope image of a liquid-crystal molecule (5-nonyl-2-nonoxylphenylpyrimidine) adsorbed on a graphite surface. (J.S. Foster, *et al.*, *Nature*, **338**, 137 (1988).



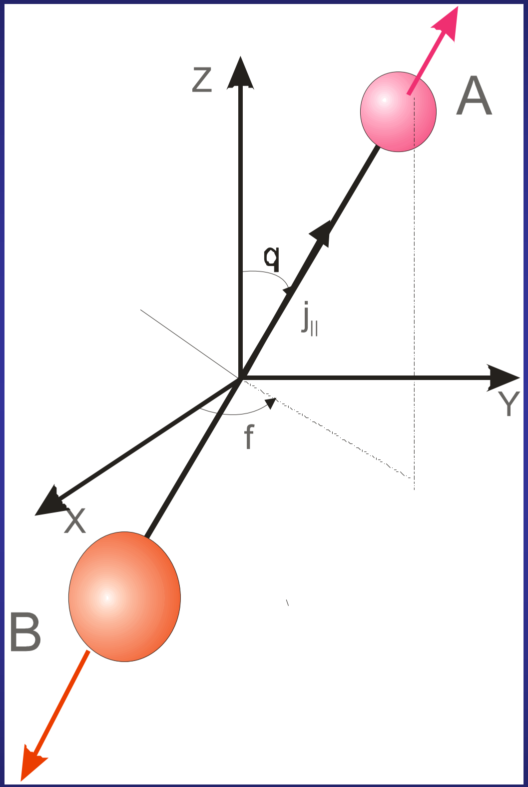
ype of image that can be obtained with a scanning tunnelling oscope. The sample is of a silicon surface and the cliff is one high. (Sang-il Park and C.F. Quaite).

Harmonic Oscillator



$F = -k\,x$

Diatomic molecule

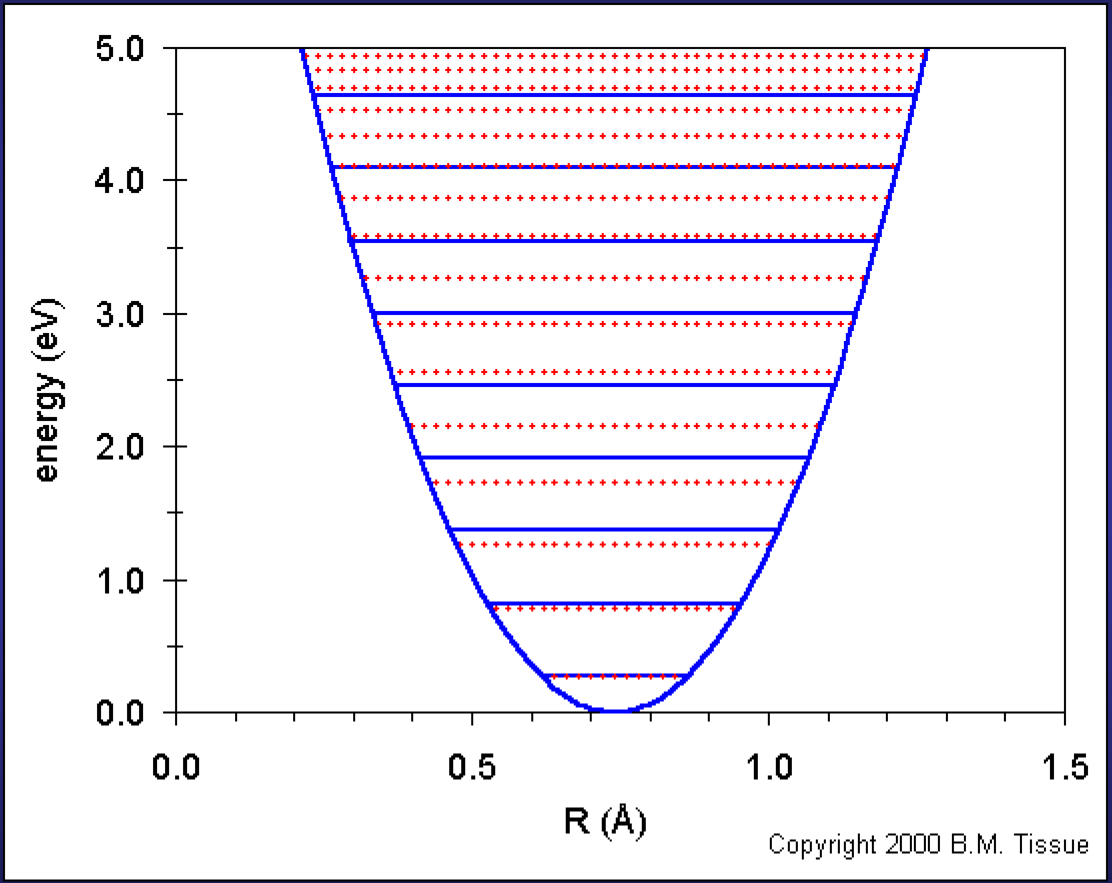


$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{kx^2}{2}\right)\psi_n(x)=E_n\psi_n(x)$$

$\mu = m_A m_B/(m_A+m_B)$

Harmonic Oscillator: Diatomic Molecule Energy Levels

$E_v = (v + ½)\,\hbar\,\omega$, $\omega = (k/\mu)^{½}$, $\mu = m_A m_B/(m_A + m_B)$

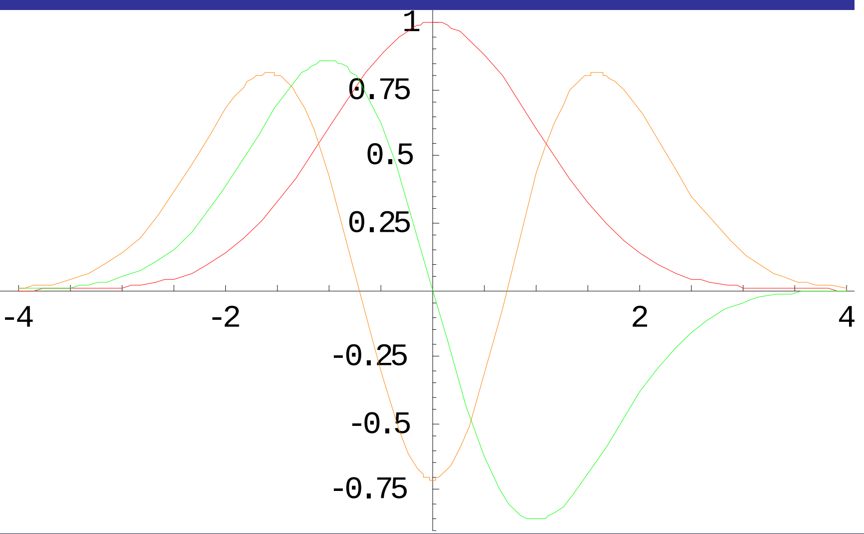


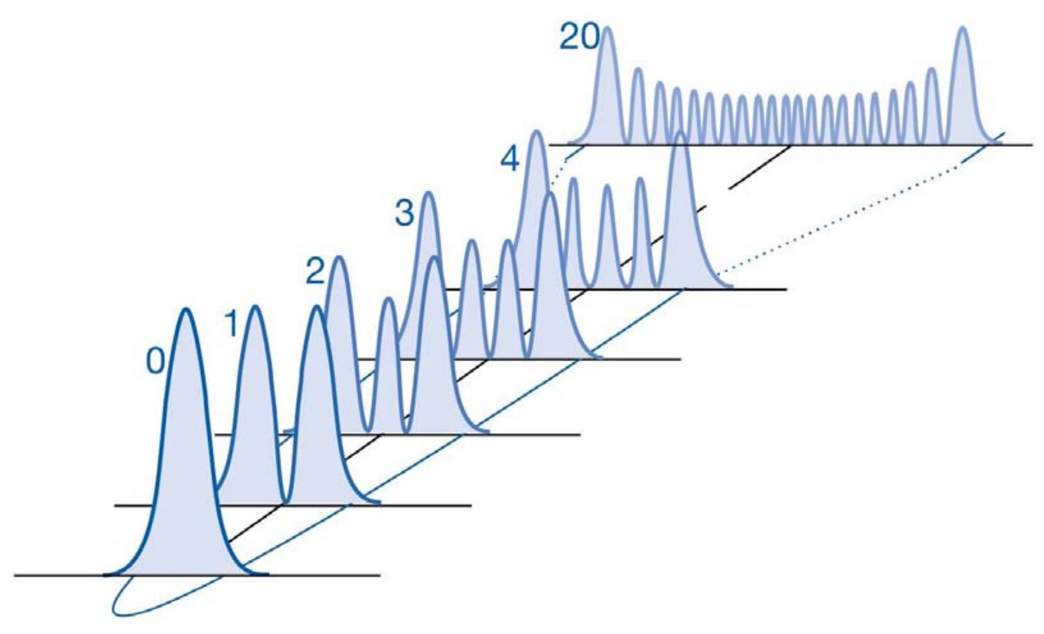
Harmonic Oscillator: the Wavefunctions

$$\psi_v(x) = N_v\, H_v(y)\, e^{-y^2/2}; \qquad y = \frac{x}{\alpha}; \qquad \alpha = \left(\frac{\hbar^2}{\mu k}\right)^{\frac{1}{4}}$$

H_v are Hermite polynomials: $H_0(y) = 1$, $H_1(y) = 2y$, $H_2(y) = 2y^2 – 2$, $H_3(y) = 8y^2 – 12y$, ets.

v = 2 1 0

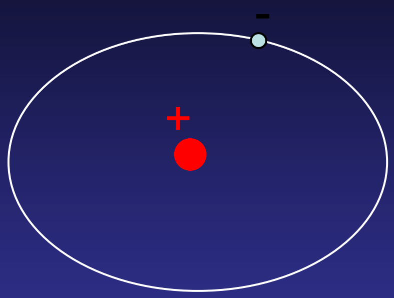




$\psi(x)$

$|\psi(x)|^2$

Hydrogen Atom

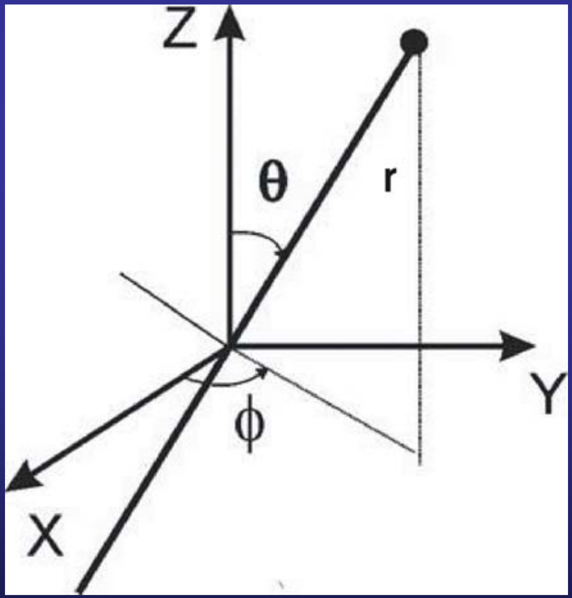


Hamiltonian

$$H\psi_k = E_k\psi_k$$

$$\boldsymbol{H} = -\frac{\hbar^2}{2\boldsymbol{m_e}}\nabla_{\boldsymbol{e}}^2 - \frac{\boldsymbol{Z}\,\boldsymbol{e}^2}{4\pi\varepsilon_0\,\boldsymbol{r}}$$

Polar coordinates



$$\nabla_{\boldsymbol{e}}^2 = \frac{\partial^2}{\partial \boldsymbol{x}^2} + \frac{\partial^2}{\partial \boldsymbol{y}^2} + \frac{\partial^2}{\partial \boldsymbol{z}^2}$$

$$\nabla_{\boldsymbol{e}}^2 = \frac{1}{\boldsymbol{r}^2}\left(\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{r}^2\frac{\partial}{\partial \boldsymbol{r}}\right) + \Lambda^2(\theta,\phi)$$

$$\Lambda^2(\theta,\phi) = \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\theta^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}$$

Wavefunctions

$$\psi_{\boldsymbol{k}}(\boldsymbol{r},\theta,\phi)$$

where **k ≡ n, l, s, m_l, m_s**

$$\psi_{\boldsymbol{k}}(\boldsymbol{r},\theta,\phi) = \boldsymbol{R}_{\boldsymbol{nl}}(\boldsymbol{r})\,\mathrm{Y}_{\boldsymbol{l}\,\boldsymbol{m}_l}(\theta,\phi)\,\chi_{\boldsymbol{s}\,\boldsymbol{m}_s}$$

$R_{n\,l}$ are Associated Laguerre polynomials and $Y_{l\,m}$ are Spherical Harmonics

Spherical Harmonics for $l = 0, 1, 2, 3, 4$

$Y_{l,m}(\theta, \phi) = P_l^m(\cos\theta) \cdot f_m(\phi) \qquad f_m(j) = {}^1/_{(2\pi)}{}^{½}\, e^{im\phi}$

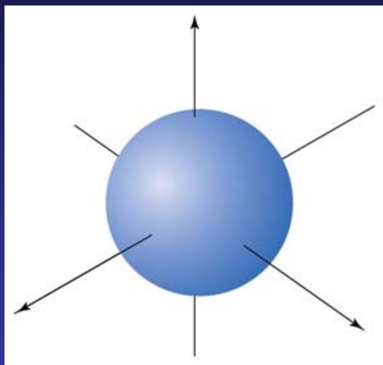
Elektron	l	m	$Y_{l,m}(\theta, \phi)$	$\lvert Y_{l,m}\rvert^2$
s	0	0	${}^1/_{(4\pi)}{}^{½}$	${}^1/_{4\pi}$
p	1	±1	$\pm({}^3/_{8\pi})^{½} \sin\theta\, e^{\pm i\phi}$	${}^3/_{8\pi} \sin^2\theta$
	1	0	$({}^3/_{4\pi})^{½} \cos\theta$	${}^3/_{4\pi} \cos^2\theta$
d	2	±2	$({}^{15}/_{32\pi})^{½} \sin^2\theta\, e^{\pm 2i\phi}$	${}^{15}/_{32\pi} \sin^4\theta$
	2	±1	$\pm({}^{15}/_{8\pi})^{½} \sin\theta \cos\theta\, e^{\pm i\phi}$	${}^{15}/_{8\pi} \sin^2\theta \cos^2\theta$
	2	0	$({}^5/_{16\pi})^{½} (3\cos^2\theta - 1)$	${}^5/_{16\pi}(3\cos^2\theta - 1)^2$
f	3	±3	$({}^{35}/_{64\pi})^{½} \sin^3\theta\, e^{\pm 3i}\,\phi$	${}^{35}/_{64\pi} \sin^6\theta$
	3	±2	$({}^{105}/_{32\pi})^{½} \sin^2\theta \cos\theta\, e^{\pm 2i\phi}$	${}^{105}/_{32\pi} \sin^4\theta \cos^2\theta$
	3	±1	$({}^{21}/_{64\pi})^{½} \sin J\, (5\cos^2\theta - 1)\, e^{\pm i\phi}$	${}^{21}/_{64\pi} \sin^2\theta\, (5\cos^2\theta - 1)^2$
	3	0	$({}^7/_{16\pi})^{½} (5\cos^3\theta - 3\cos\theta)$	${}^7/_{16\pi} (5\cos^3\theta - 3\cos\theta)$
g	4	±4	$({}^{315}/_{512\pi})^{½} \sin^4\theta\, e^{\pm i4\phi}$	${}^{315}/_{512\pi} \sin^8\theta$
	4	±3	$({}^{315}/_{64\pi})^{½} \sin^3\theta \cos\theta\, e^{\pm 3i\phi}$	${}^{315}/_{64\pi} \sin^6\theta \cos^2\theta$
	4	±2	$({}^{225}/_{660\pi})^{½} \sin^2\theta\, (7\cos^2\theta - 1)\, e^{\pm 2i\phi}$	${}^{225}/_{660\pi} \sin^4\theta\, (7\cos^3\theta - 1)^2$
	4	±1	$({}^{225}/_{320\pi})^{½} \sin J\, (7\cos^3\theta - 3\cos\theta)\, e^{\pm i\phi}$	${}^{225}/_{320\pi} \sin^2\theta\, (7\cos^3\theta - 3\cos\theta)^2$
	4	0	$({}^9/_{256\pi})^{½} (35\cos^4\theta - 30\cos^2\theta + 3)$	${}^9/_{256\pi} (35\cos^4\theta - 30\cos^2\theta + 3)^2$

Real Wavefunctions Obtained from Linear Combinations

l	$\lvert m_l \rvert$	Wavefunctions
0	0	$s = {}^{1}/_{(4\pi)}{}^{1/2}$
1	0	$p_z = ({}^{3}/_{4\pi})^{1/2} \cos\vartheta$
	1	$p_x = ({}^{3}/4\pi)^{1/2} \sin\vartheta \cos\varphi$
		$p_y = ({}^{3}/_{4\pi})^{1/2} \sin\vartheta \sin\varphi$
2	0	$d_{3z^2-r^2} = ({}^{5}/_{16\pi})^{1/2}(3\cos^2\vartheta - 1)$
	1	$d_{xz} = ({}^{15}/_{4\pi})^{1/2} \sin\vartheta \cos\vartheta \cos\varphi$
		$d_{yz} = ({}^{15}/_{4\pi})^{1/2} \sin\vartheta \cos\vartheta \sin\varphi$
	2	$d_{x^2-y^2} = ({}^{15}/_{16\pi})^{1/2} \sin^2\vartheta \cos\varphi$
		$d_{xy} = ({}^{15}/_{16\pi})^{1/2} \sin^2\vartheta \sin\varphi$

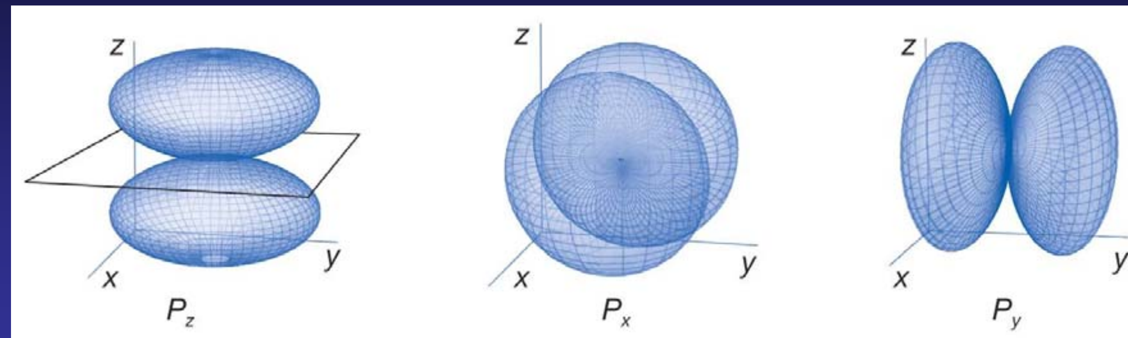
Hydrogen Atom Wavefunctions: Angular Part

s orbital:
l = 0 m = 0

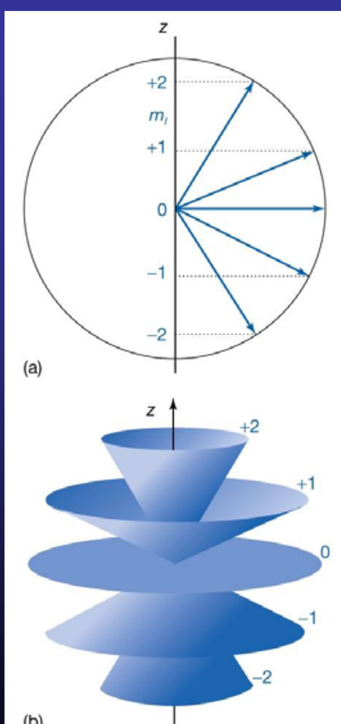


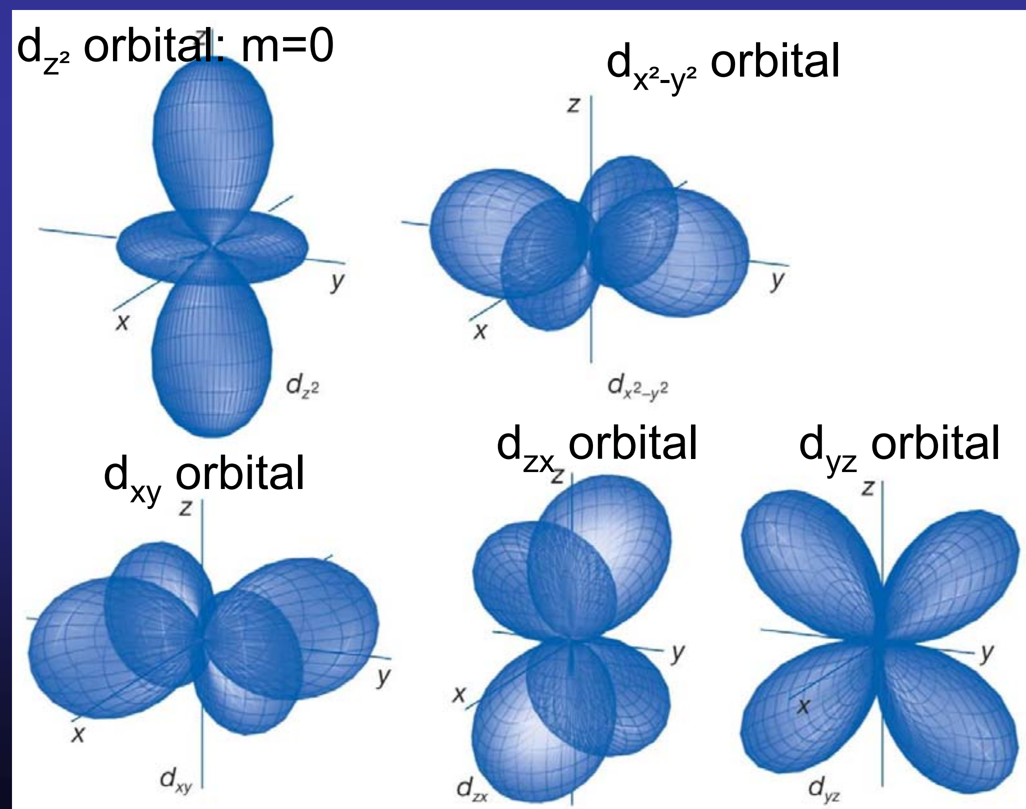
p_Z orbital: p_X orbital p_Y orbital

l = 1 m = 0 **l = 1 m = ±1**

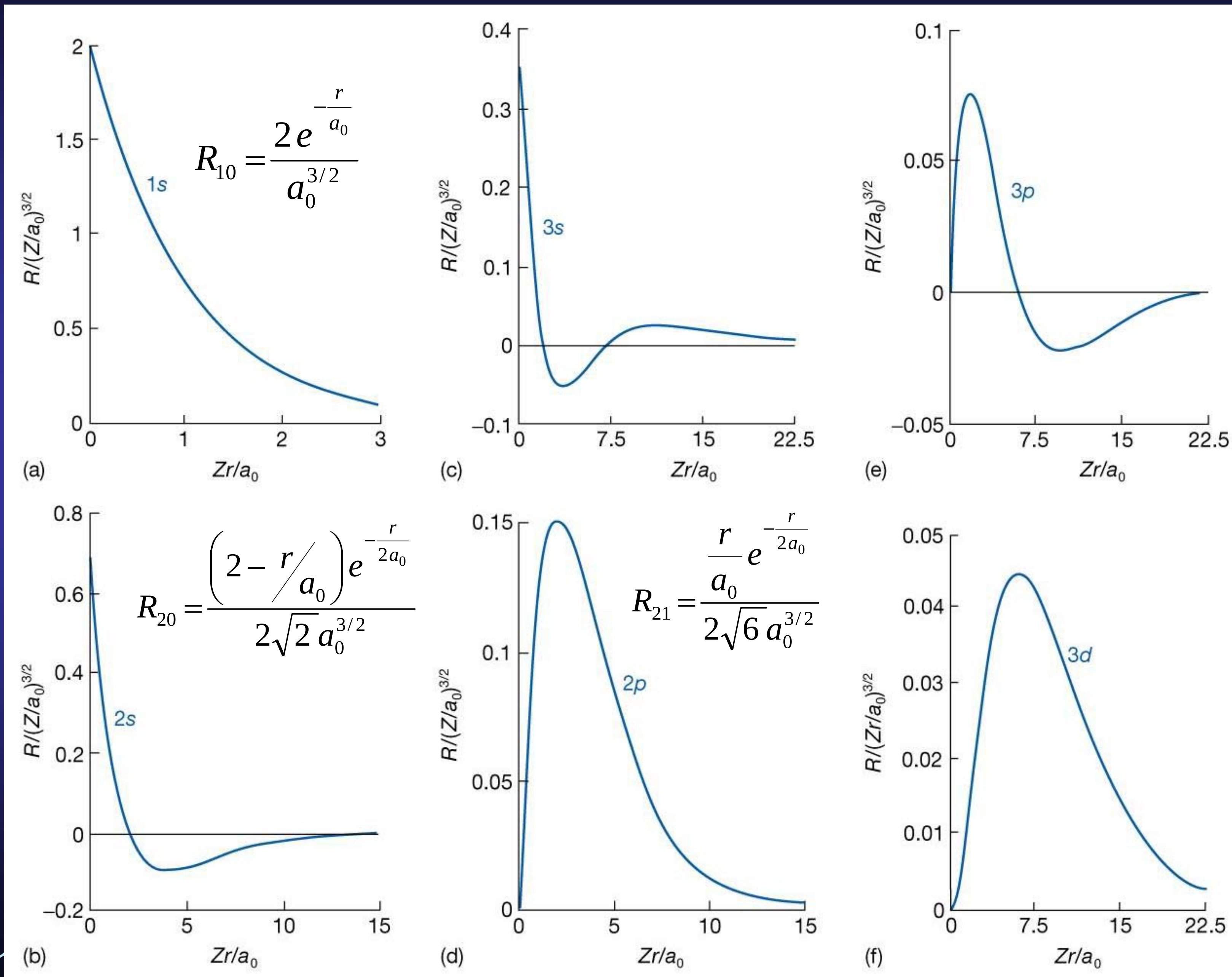


l = 2





Hydrogen Atom Wavefunctions: Radial Part



$$R_{10} = \frac{2e^{-\frac{r}{a_0}}}{a_0^{3/2}}$$

$$R_{20} = \frac{\left(2 - \frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}}{2\sqrt{2}\,a_0^{3/2}}$$

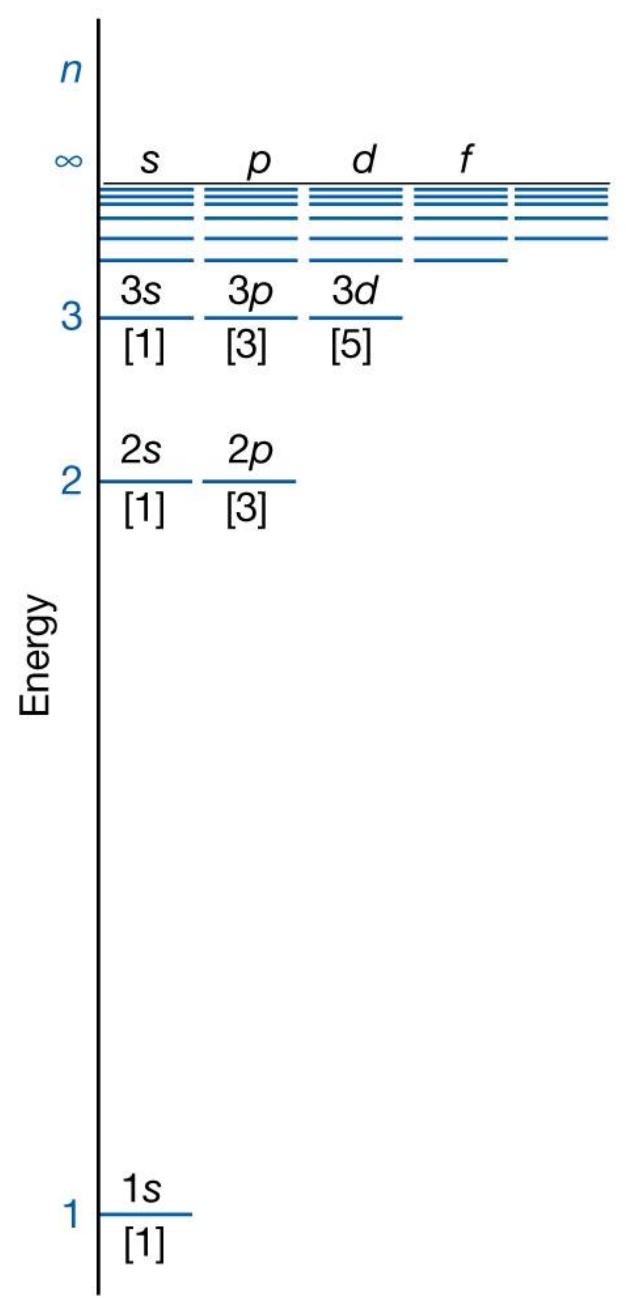
$$R_{21} = \frac{\frac{r}{a_0}e^{-\frac{r}{2a_0}}}{2\sqrt{6}\,a_0^{3/2}}$$

Niels Henrik David **Bohr**

* 7. Okt. 1885 in Kopenhagen,
+ 18. Nov. 1962 in Kopenhagen

Nobelpreis 1965

Hydrogen Atom Energy Levels



$$E_{nl} = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{2a_0 n^2} \qquad n = 1, 2, 3, \ldots$$

ε_0 is the Vacuum permittivity; $\varepsilon_0 = 8.854 \cdot 10^{-12}$ J^{-1} C^2 m^{-1}

e is the Elementary charge; $e = 1.602 \cdot 10^{-19}$ C

a_0 is the Bohr radius; $a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2 = 5.292 \cdot 10^{-11}$ m