Kým bude reč o elektrónovej štruktúre atómov ...

Častica

diskrétna jednotka hmoty

hmotnosť + hybnosť

kinetická energia

elektrický náboj
(nemusí mať)

Vlna

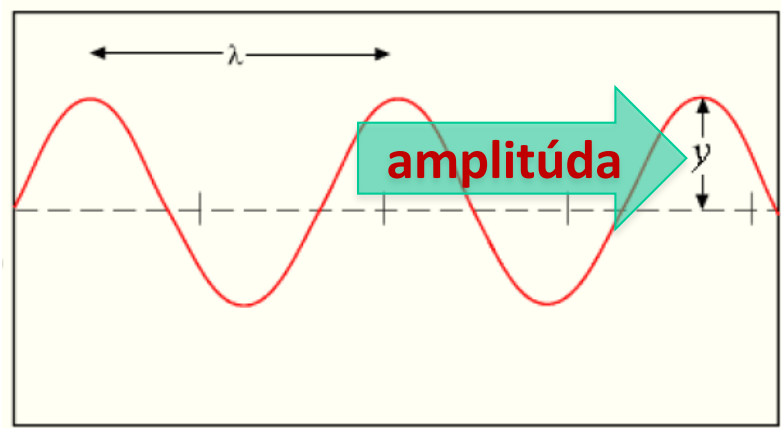
periodická zmena veličiny
-funkcia lokality alebo času

$$\lambda = \frac{u}{\nu}$$

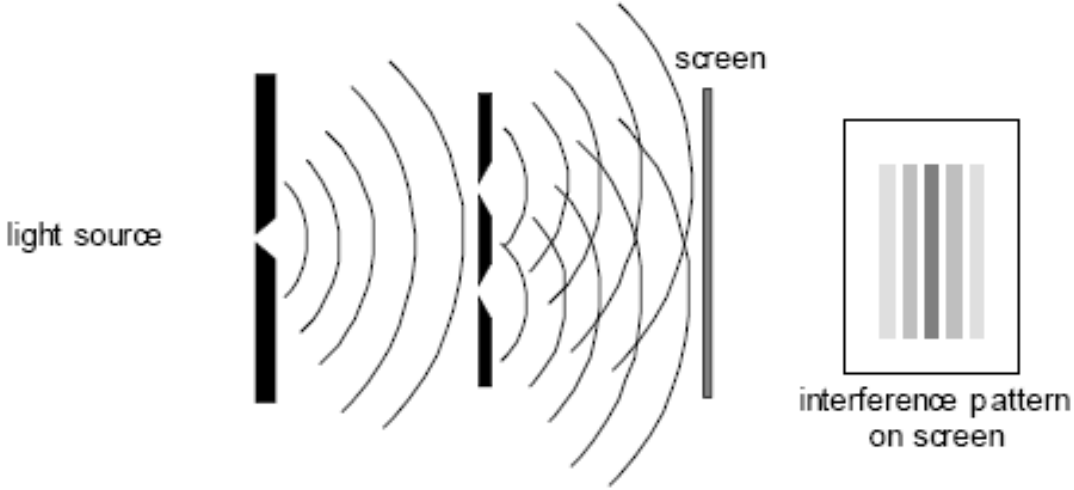
u ← rýchlosť šírenia

ν ← frekvencia

λ ← vlnová dĺžka



Čo je svetlo?

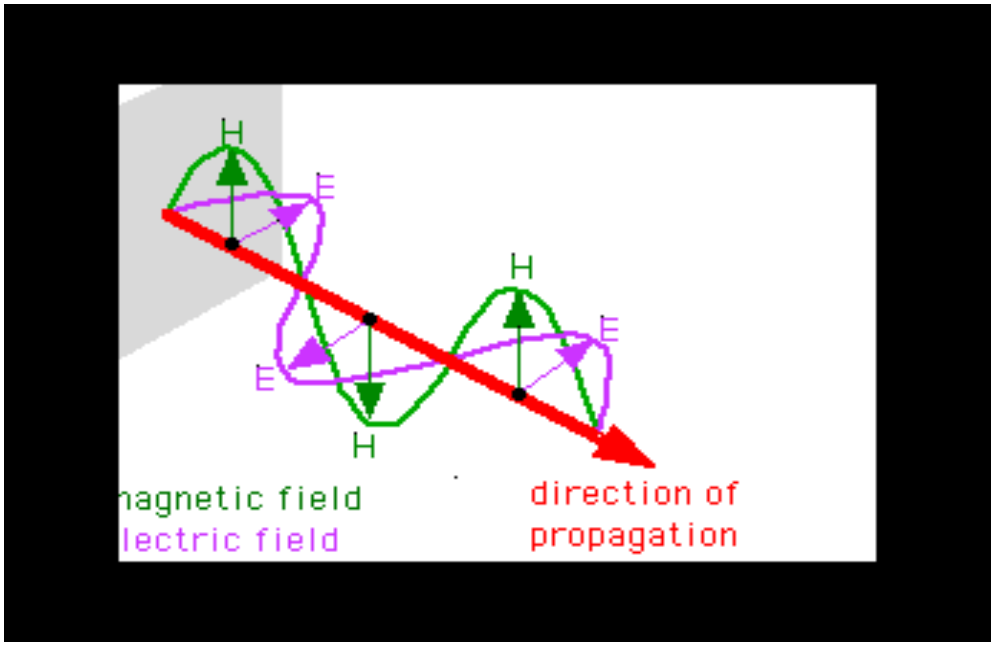


19 storočie

Thomas Young

efekt interferencie

vlnenie



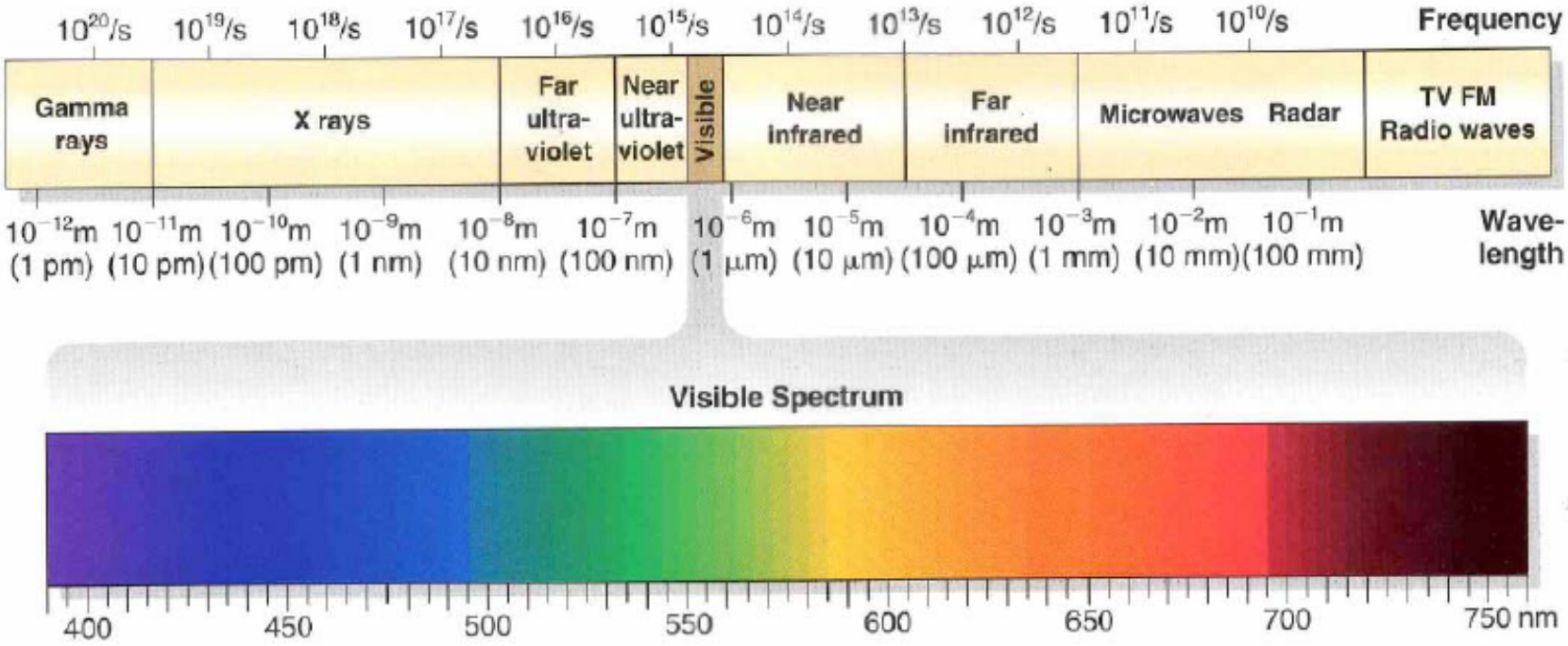
James Clerk Maxwell

Škót, 1860

elektromagnetická teória

$$\nu = c/\lambda$$

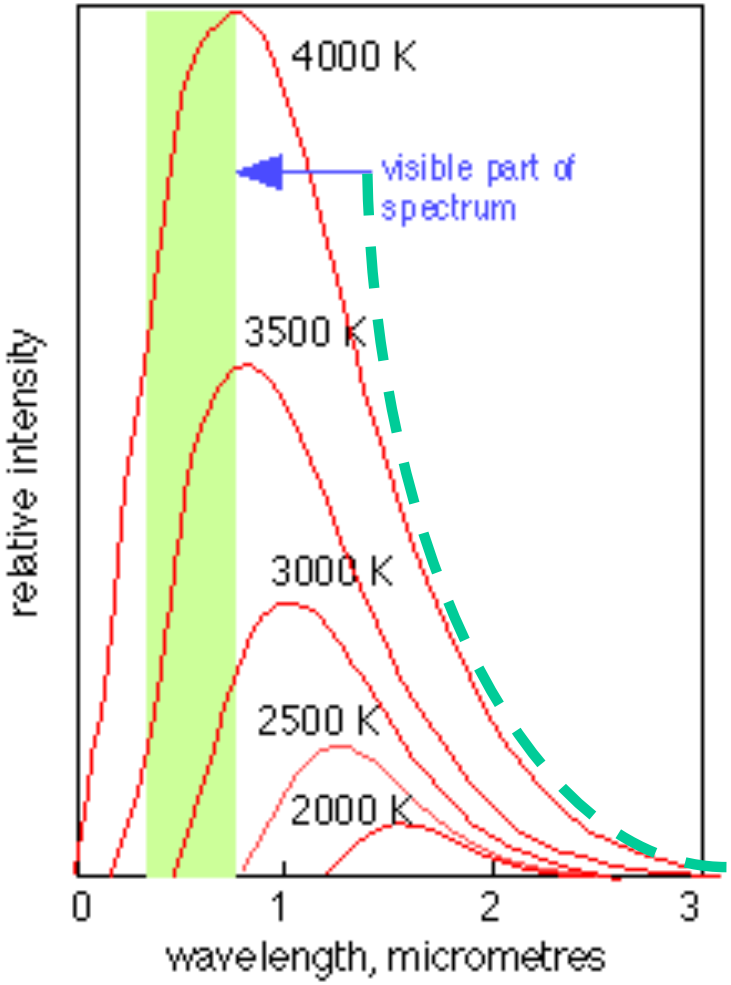
Elektromagnetické žiarenie



Vysoká Energia

Nízka Energia

Čo zostávalo nevysvetlené ...



Žiarenie (absolútne čierneho) telesa

Wilhelm Wien – empiricky

λ_{max}(cm)=0.29/T

klasicky $$I(\lambda) = \frac{8\pi kT}{\lambda^4}$$

Max Planck (1858-1947) – Nemec

1918 – Nobelova cena

oscilátory vymieňajú s okolím energiu v kvantách hν

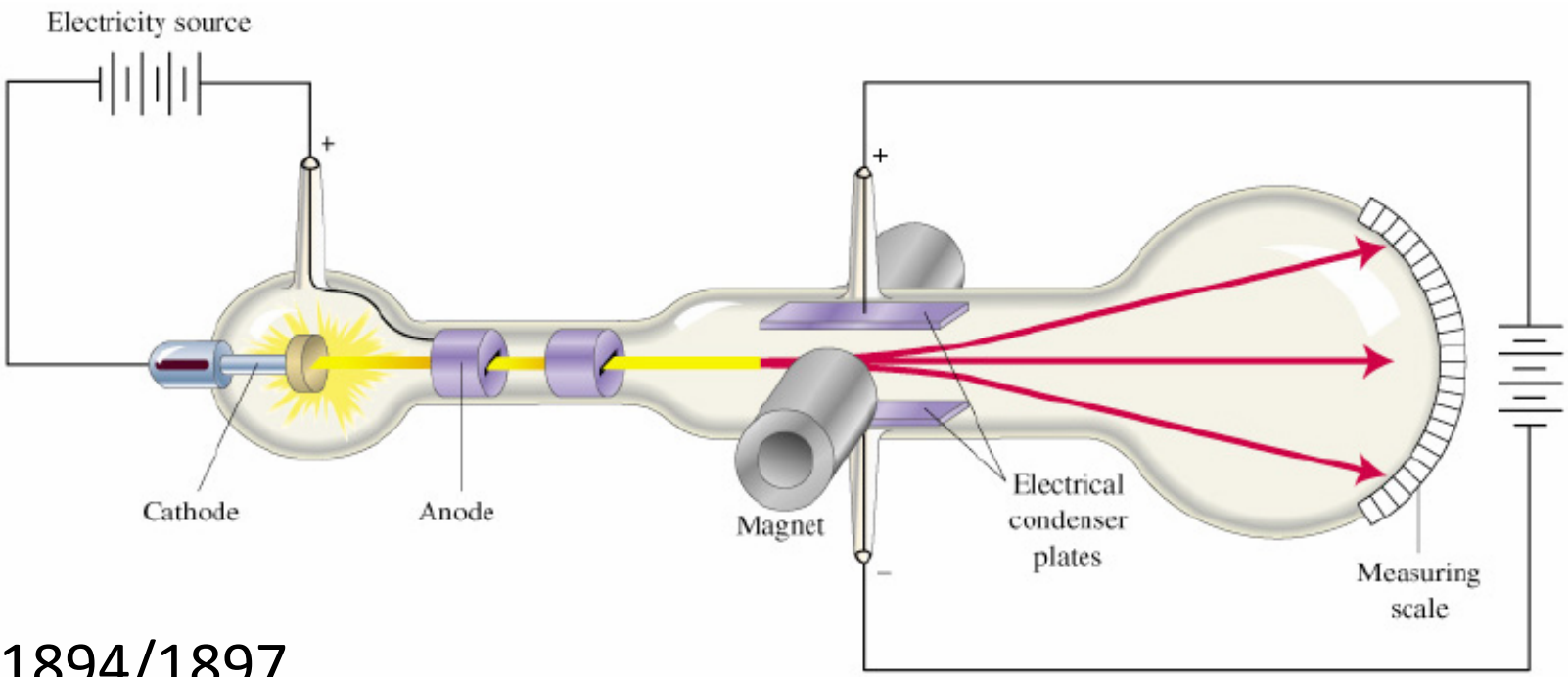
$h=6.626\times10^{-34}$ Js

Planckova konštanta

$$\frac{2\pi hc^2}{\lambda^5}\frac{1}{e^{hc/\lambda kT}-1}$$

Joseph John Thomson, 1856-1940 Nobelova cena 1906

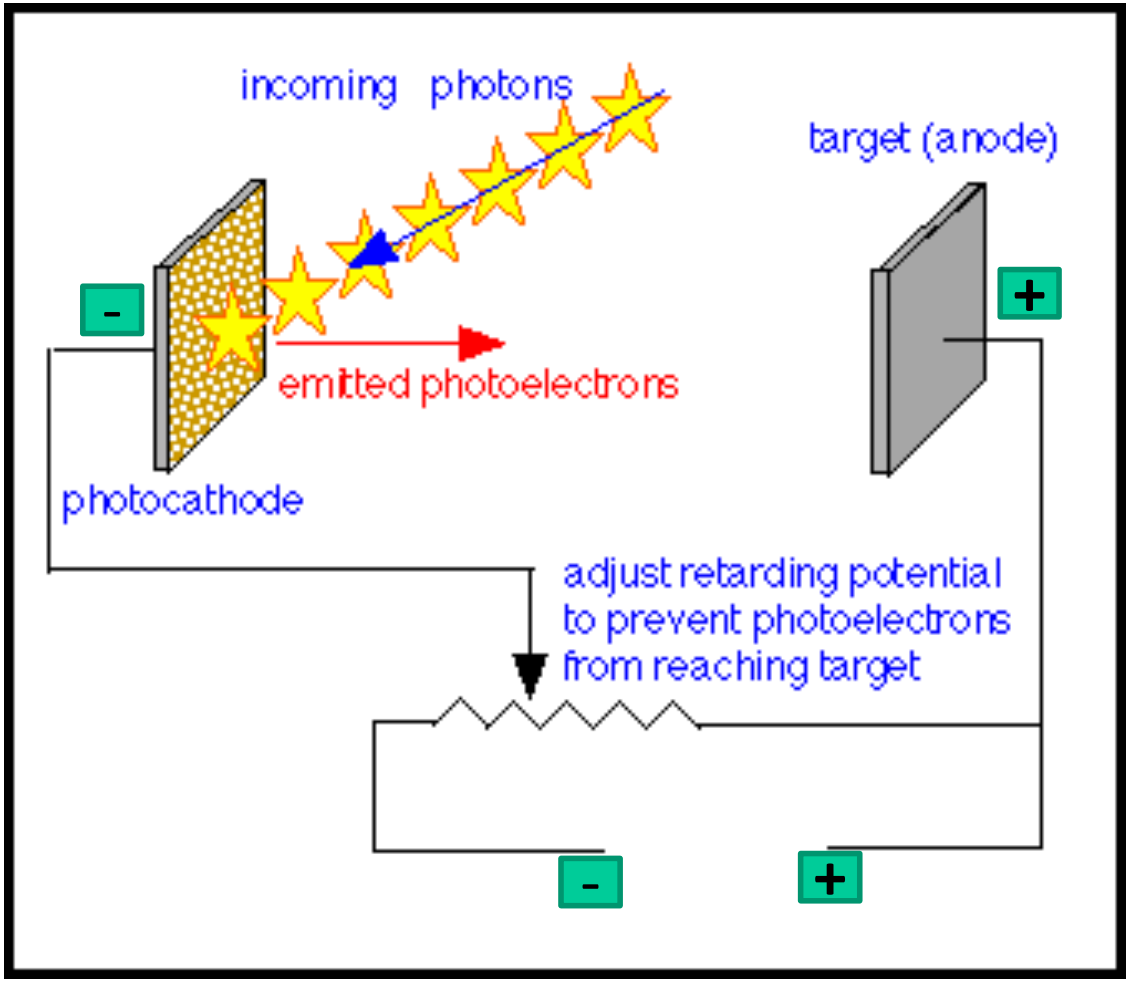
Thomsonov experiment



1894/1897

Dá sa určiť pomer hmotnosti a náboja elektrónu $e/m = -1.76.10^8$ C/g

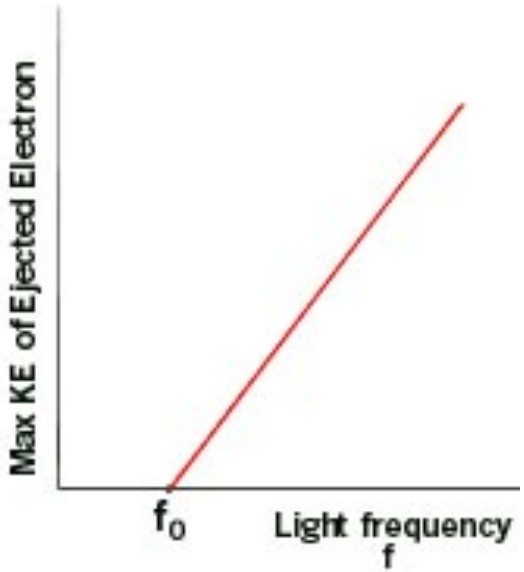
Čo je fotoelektrický jav?



retardačný potenciál

- zastaví tok elektrónov

$$V_r e = m v^2/2$$



Kinetická energia nezávisí od intenzity ožarovania!!!!

Albert Einstein

$$\varepsilon = h\nu = \frac{hc}{\lambda}$$

Ak mal Planck pravdu, potom aj každý „balík“ svetla musí byť skoncentrovaný v malej oblasti na čele vlny → **kvantovaná častica**

$$m_v = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

m_0 – pokojová hmotnosť

v – rýchlosť

c – rýchlosť svetla

fotón

Ak sa má niečo pohybovať rýchlosťou svetla, musí mať nulovú pokojovú hmotnosť

A čo hybnosť? ($\vec{p}=m\vec{v}$)

$$\varepsilon = mc^2 \qquad \frac{h\upsilon}{c^2} \times c = \frac{h\upsilon}{c} = \frac{h}{\lambda}$$

Louis de Broglie, Francúz

Ak svetlo má charakter častice → častica má charakter vlny

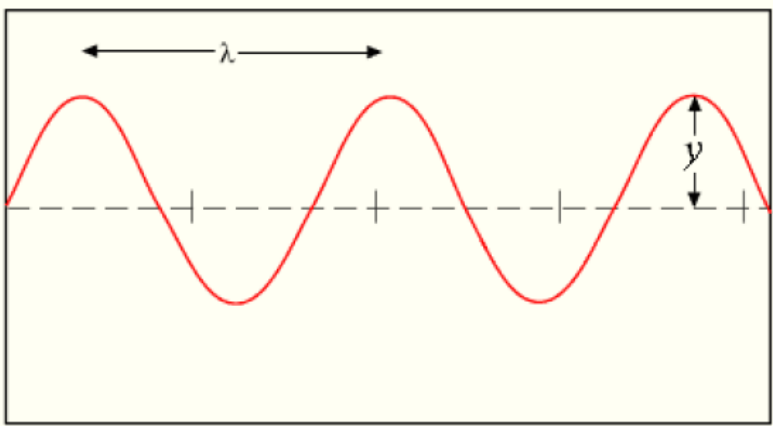
1924 Dr. práca

$$\lambda = h/mv = h/p$$

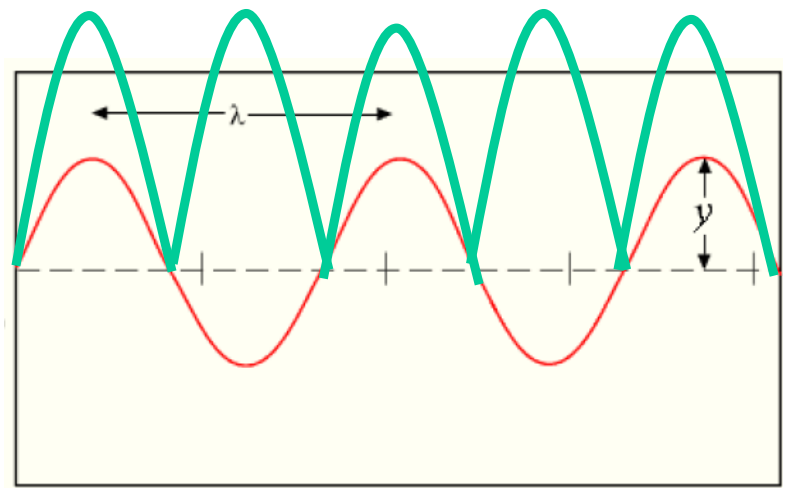
1927 – Bell laboratóriá
ohyb elektrónov na niklovej fólii

1929 - Nobelova cena

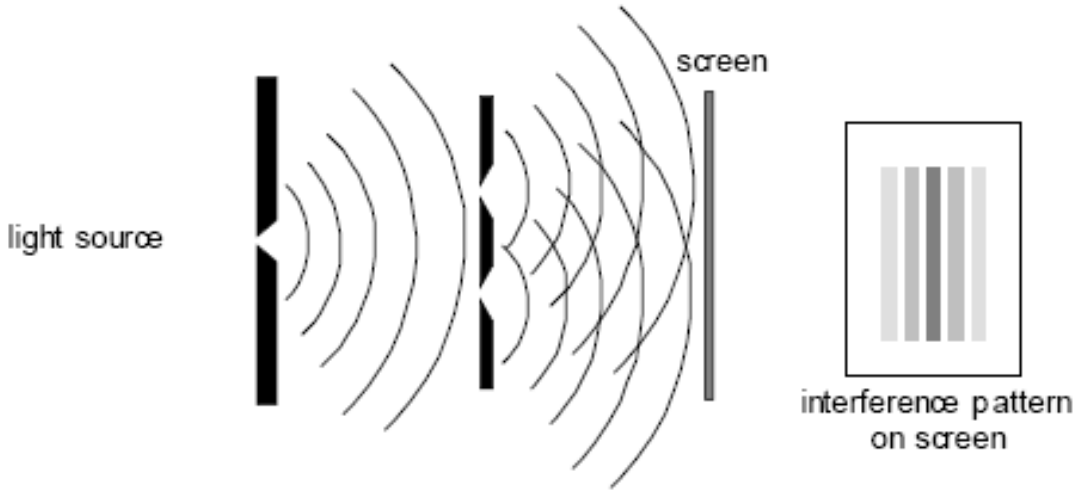
Čo je vlnenie (inak)



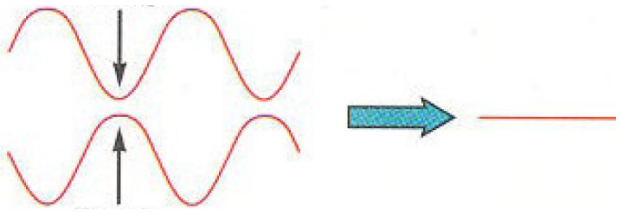
Hodnota veličiny, ktorej štvorec je mierou pravdepodobnosti výskytu častice v danej lokalite



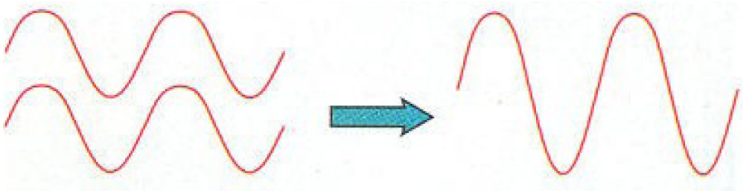
matematická (pravdepodobnostná) funkcia



deštruktívna interferencia



konštruktívna interferencia



1927 Werner Heisenberg (Nemec)
– princíp neurčitosti

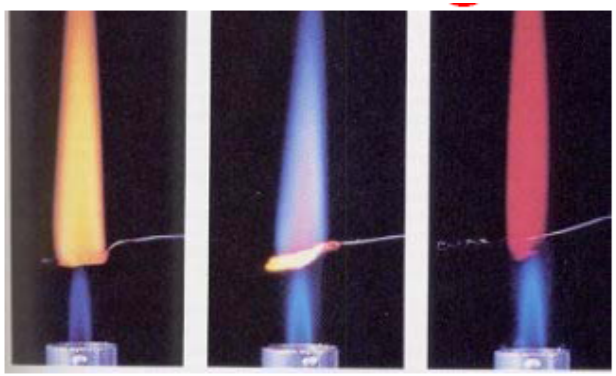
Niektoré dvojice veličín nemožno určiť (spoločne) s ľubovoľnou presnosťou.

$$\Delta p \cdot \Delta x \geq \hbar/2$$

$$\hbar = h/2\pi$$

$$\Delta E \cdot \Delta t \geq \hbar/2$$

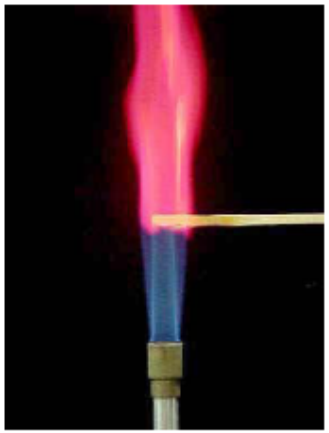
A čo atóm a elektróny v ňom?



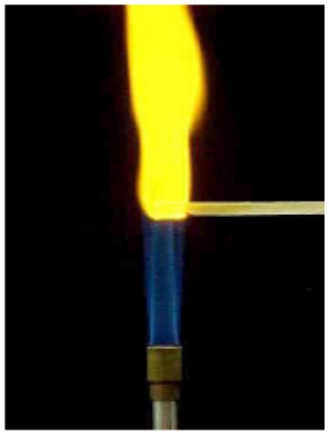
Na K Li

CH_4

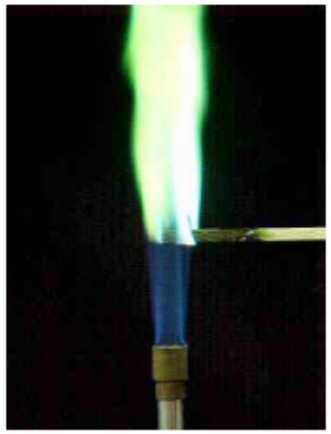
Wood



Sr



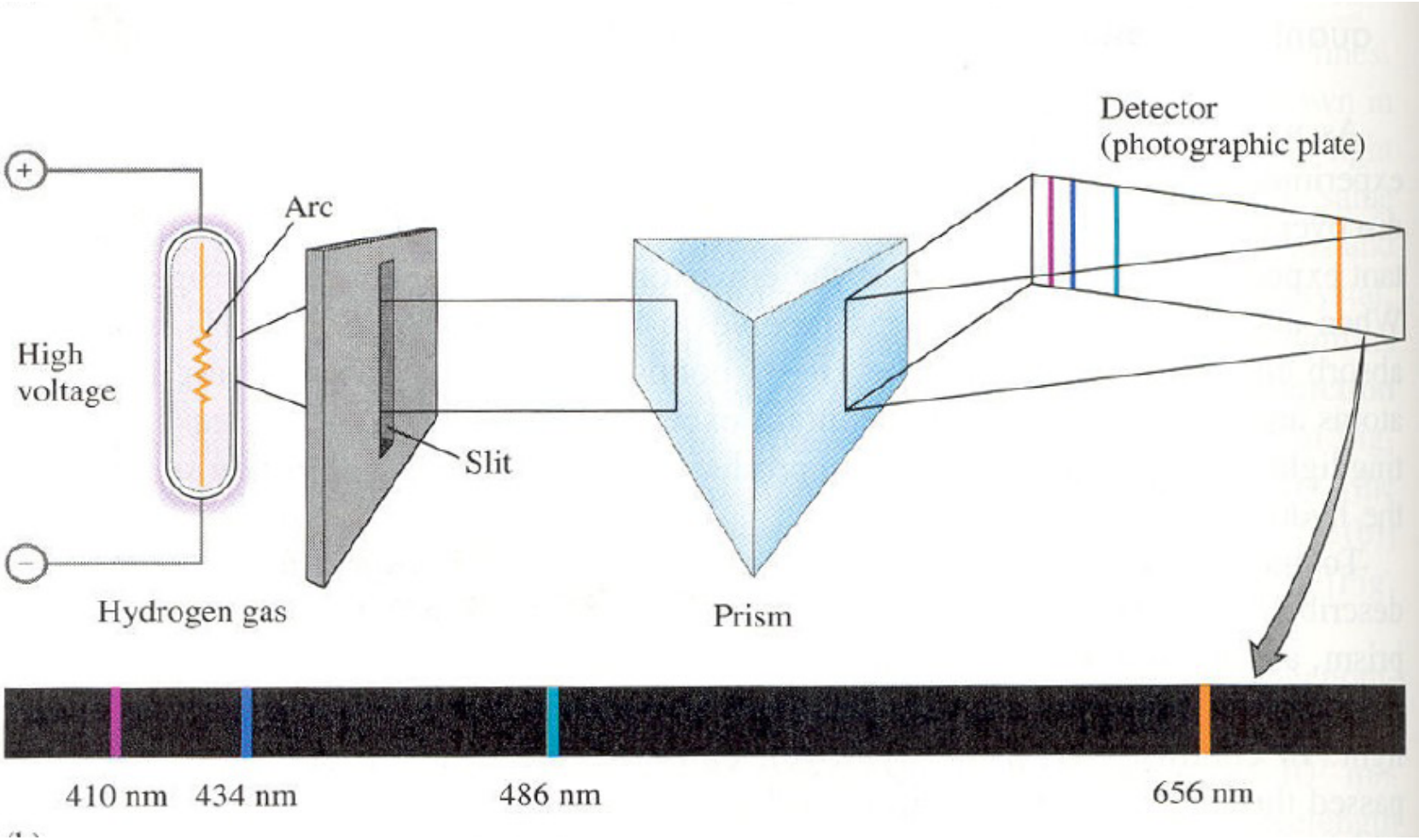
Na



Cu

Ca

Čo je čiarové spektrum?



Vodík

Spektrum vodíka

Série (UV, vis, IR)

Švajčiarsky učiteľ Balmer

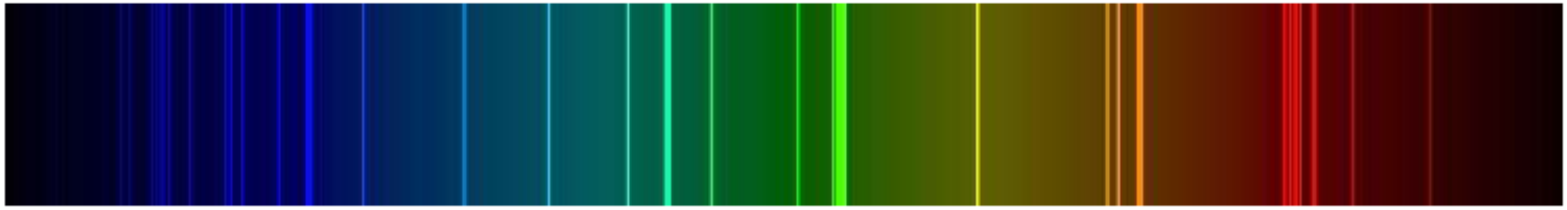
$$\frac{1}{\lambda} = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

$R = 109737\ cm^{-1}$

Name of series	when discovered	value of *m*
Lyman	1906-14	1
Balmer	1885	2
Paschen	1908	3
Brackett	1922	4
Pfund	1924	5

Príklady emisných spektier

Ca

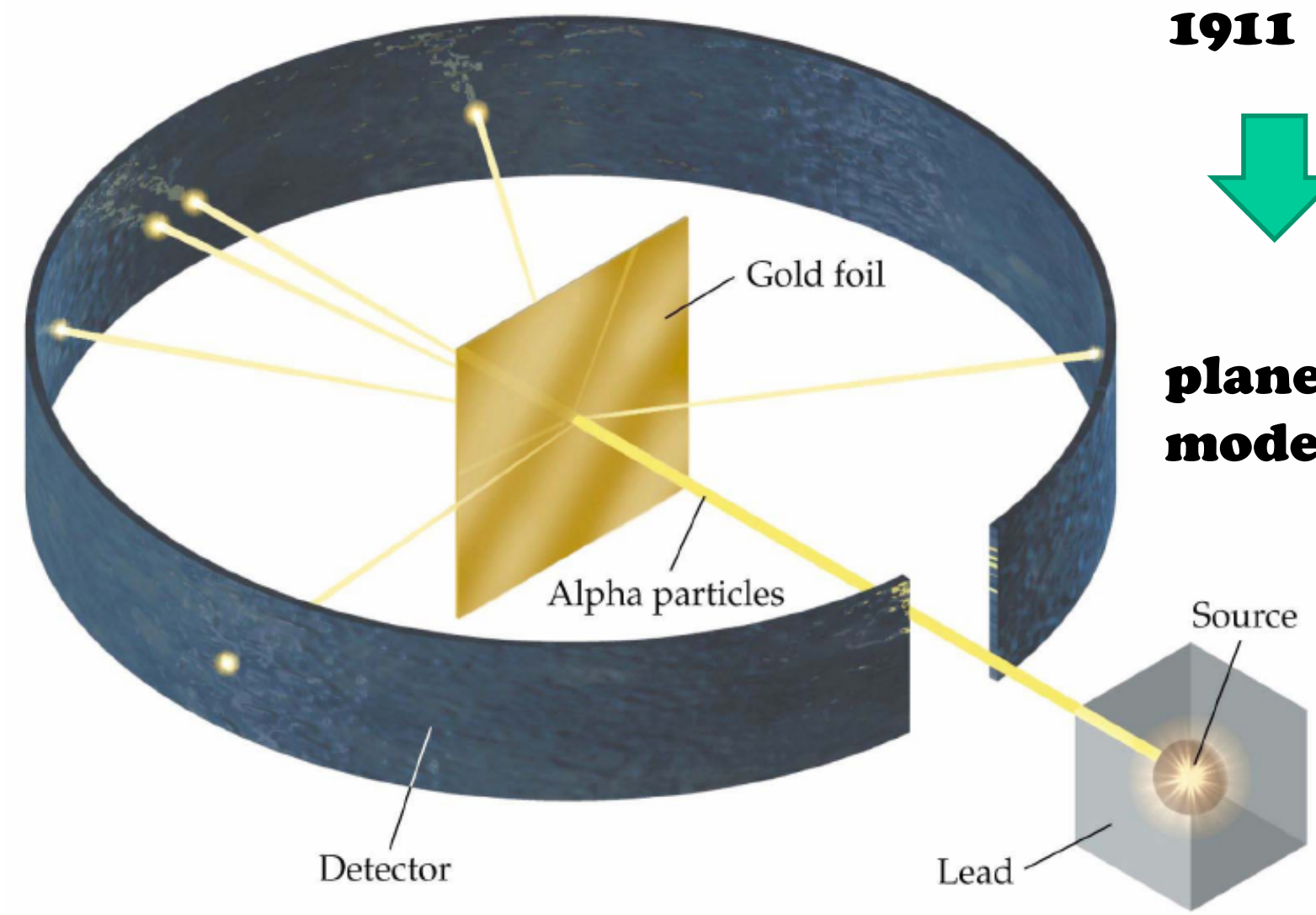


Na

Cu

Ba

Rutherfordov experiment

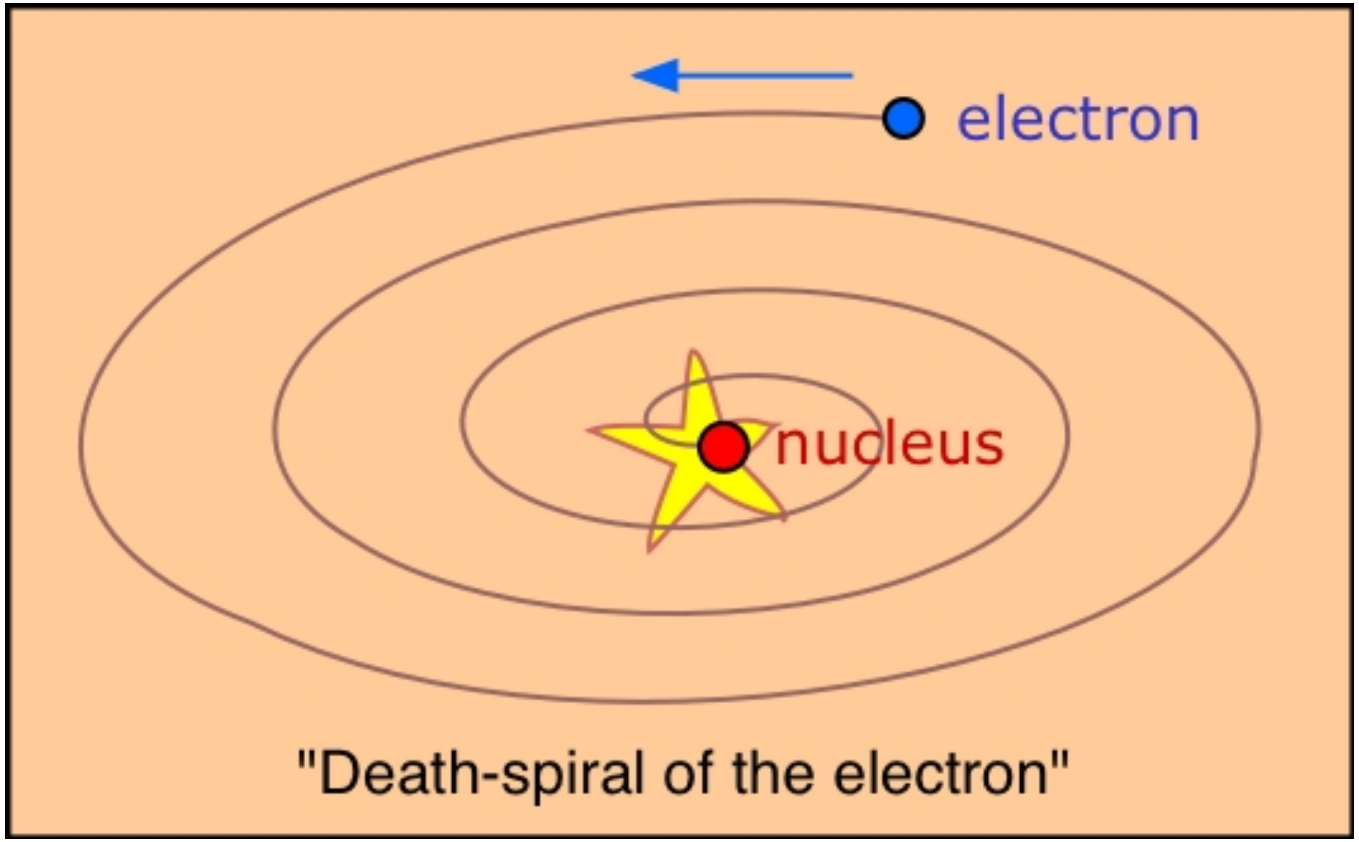


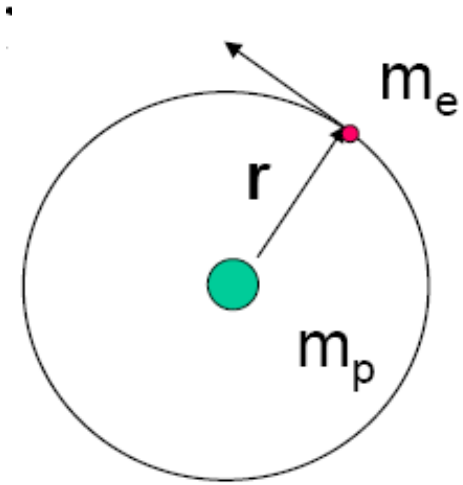
1911

planetárny model

Ernest Rutherford, 1881-1937

Defekt planetárneho modelu





$$E=-e^2/(8\pi\varepsilon_0 r)$$

Niels Bohr, Dán, 1913 – Bohrov model

(kombinácia s Planckovou teóriou)

$$2\pi rmv = nh$$

$$E_n = -\frac{m_e e^4}{8\varepsilon_o^2 n^2 h^2} = -\frac{me^4}{8\varepsilon_o^2 h^2}\frac{1}{n^2}$$

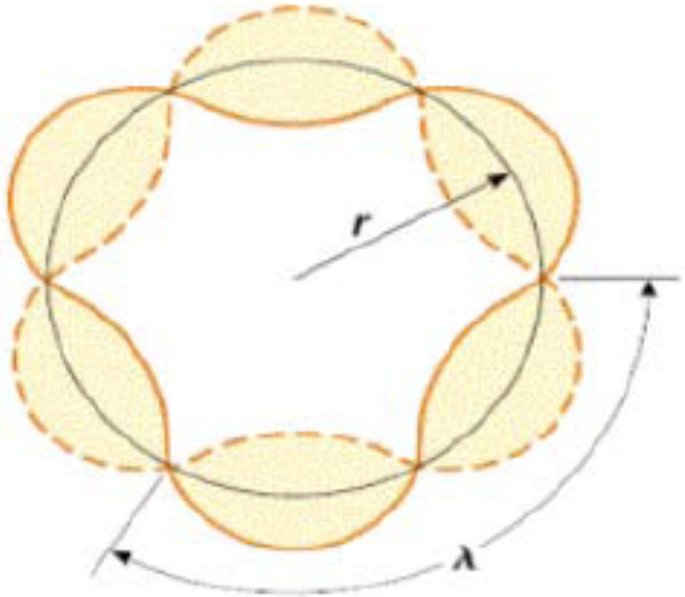
$$r = \frac{n\hbar^2}{m_e e^2}$$

$$\Delta E = E_{n_1} - E_{n_2} = konst\left(\frac{1}{n_2^{\,2}} - \frac{1}{n_1^{\,2}}\right)$$

$$a_0 = 0.529 \text{ Å}$$

Bohrov polomer

O pár rokov neskôr – kombinácia s De Broglie záchrana modelu



náboj je stacioárny!

Mechanika

klasická versus kvantová

trajektória pohyb **vlna**

hybnosť

$$\lambda = h/mv = h/p$$

vlnová funkcia

$$\Psi(x,t)$$

$$\Psi^*(x,t) \cdot \Psi(x,t)$$

$$|\Psi(x,t)|^2$$

pravdepodobnosť výskytu častice v bode *x* v čase *t*

bleskové repetitórium matematiky

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

$$f(x) \longrightarrow f(x,y,z)$$

$$\frac{\partial f(x,y,z)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x,y,z) - f(x,y,z)}{\Delta x}$$

$$\frac{\partial f(x,y,z)}{\partial y} = \lim_{\Delta y \to 0} \frac{f(x,y+\Delta y,z) - f(x,y,z)}{\Delta y}$$

$$\frac{\partial f(x,y,z)}{\partial z} = \lim_{\Delta z \to 0} \frac{f(x,y,z+\Delta z) - f(x,y,z)}{\Delta z}$$

$$\nabla f = \mathbf{x}_u \frac{\partial f}{\partial x} + \mathbf{y}_u \frac{\partial f}{\partial y} + \mathbf{z}_u \frac{\partial f}{\partial z}$$

$$\nabla = \mathbf{x}_u \frac{\partial}{\partial x} + \mathbf{y}_u \frac{\partial}{\partial y} + \mathbf{z}_u \frac{\partial}{\partial z}$$

Vektor!

Laplaceov operátor

$$\triangle = \nabla . \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

skalárny súčin: a.b = |a|.|b| cos(α)

$$\mathbf{x}_u \mathbf{y}_u = \mathbf{x}_u \mathbf{z}_u = \mathbf{y}_u \mathbf{z}_u = 0$$

Vlastnosti vlnovej funkcie

Jednoznačnosť, konečnosť

spojitosť → existencia prvej a druhej derivácie

žiadna singularita – môžu byť hroty

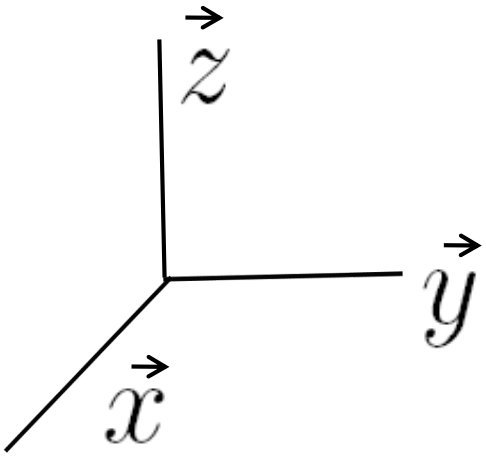
$$\int_{-\infty}^{\infty} |\Psi|^2 \, dV = 1$$

$$\frac{V}{N} \sum_{i}^{N \to \infty} |\Psi(x_i)|^2 = 1$$

Mechanika

klasická

pozorovateľná veličina



$$\vec{p} = m\vec{v}$$

kvantová

operátor

$$\hat{x} \qquad \hat{y} \qquad \hat{z}$$

$$x.\mathbf{x}_u \quad y.\mathbf{y}_u \quad z.\mathbf{z}_u$$

nabla operátor

$$\hat{p} = \frac{\hbar}{i}\nabla = -i\hbar\nabla$$

Schrödingerova rovnica

(stacionárna)

Hamiltonián
(Hamiltonov operátor)

$$\hat{H}\Psi = E\Psi$$

vlnová funkcia

energia

$$\hat{H} = \hat{H}_k + \hat{H}_p \qquad E = E_k + E_p$$

$$E_k = \frac{1}{2}mv^2 \qquad \vec{p} = m\vec{v} \quad \Rightarrow \quad E_k = \frac{\vec{p}.\vec{p}}{2m}$$

$$\hat{H}_k = \frac{\hat{p}\bullet\hat{p}}{2m} \qquad \hat{p} = -i\hbar\nabla \quad \Rightarrow \quad \hat{H}_k = -\frac{\hbar^2}{2m}\Delta$$

$$\hat{H}_p = V(x, y, z)$$

Voľný elektrón

$$\hat{p}_x = -i\hbar \mathbf{x}_u \frac{\mathrm{d}}{\mathrm{d}x} \quad \Rightarrow \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} + V(x)\Psi = E\Psi$$

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = -\frac{2m}{\hbar^2}\{E - V(x)\}\Psi \ = -k^2\Psi$$

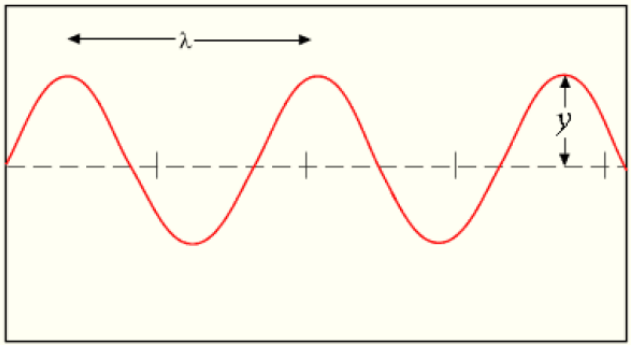
$V(x) = V$ konštantný potenciál $\qquad k = \sqrt{\dfrac{2m(E-V)}{\hbar^2}}$

$$\boxed{\Psi = \mathrm{e}^{ikx} = \cos kx + i \sin kx}$$

$$\Psi = \mathrm{e}^{ikx}$$

$$e = \lim_{n\to\infty}(1 + 1/n)^n$$

$$e = 2.718281828459045235360287471352 7 \text{ (a viac ...)}$$



$$\cos(2\pi x/\lambda)$$

$$\sin(2\pi x/\lambda)$$

$$\mathrm{e}^{i(2\pi x/\lambda)}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{ikx} = ik\mathrm{e}^{ikx}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\mathrm{e}^{ikx} = ik\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{ikx} = -k^2\mathrm{e}^{ikx}$$

rovinná vlna
(plane wave)

k – ľubovoľná hodnota

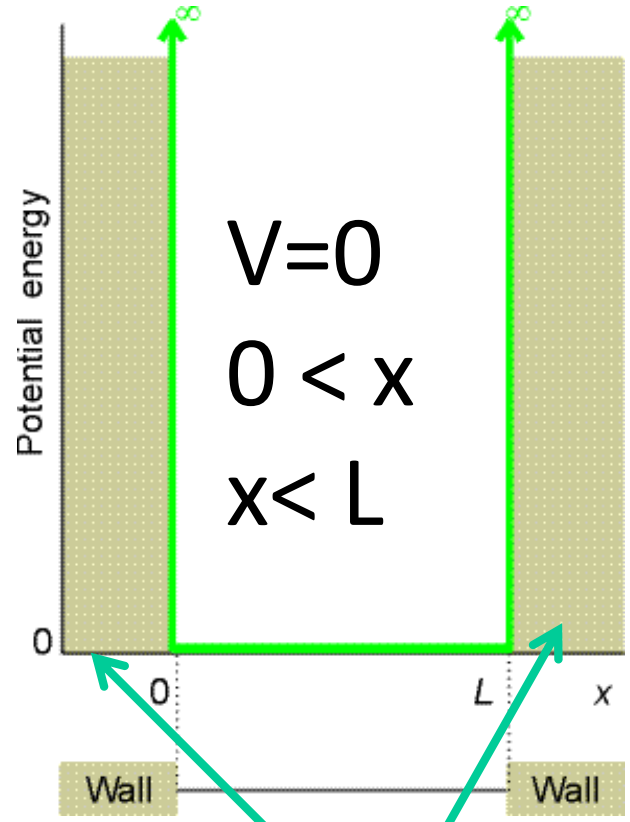
Častica v jednorozmernej potenciálovej jame (nekonečne hlbokej krabici)

$$\hat{H}_k \Longleftrightarrow \hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} = E\Psi$$

$$\Psi_k = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}$$

$$k = \sqrt{\frac{2m\ E}{\hbar^2}}$$



V=0

0 < x

x< L

V=∞

x ≤ 0; x ≥ L

$$\Psi_k = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}$$

$$\Psi_k = A\cos(kx) + iA\sin(kx) + B\cos(-kx) + iB\sin(-kx)$$

$$\cos(kx) = \cos(-kx) \qquad \sin(-kx) = -\sin(kx)$$

C,D (aj) komplexné

$$\Psi_k = C\sin(kx) + D\cos(kx)$$

Obmedzujúce podmienky: (okrajové)

$$x = 0 \Rightarrow \Psi_k(0)$$

$$\Psi_k(L) = 0$$

$$\Psi_k^*(x)\Psi_k(x) \longrightarrow \Psi_k^2$$

$$\int_0^L \Psi_k^2 dx = 1$$

$$\Psi_k = C\sin(kx) + \cancel{D\cos(kx)}$$

$$x = 0 \Rightarrow \Psi_k(0) = D \quad \Rightarrow \quad D = 0$$

$$\Psi_k(L) = 0 \Rightarrow \sin(kL) = 0 \quad \Rightarrow \quad kL = n\pi$$

$$n = 1, 2, \ldots$$

ak *n*=0 $\Rightarrow$ $\cancel{\Psi_k(x) = 0}$

nefyzikálne!

$$k = n\pi/L$$

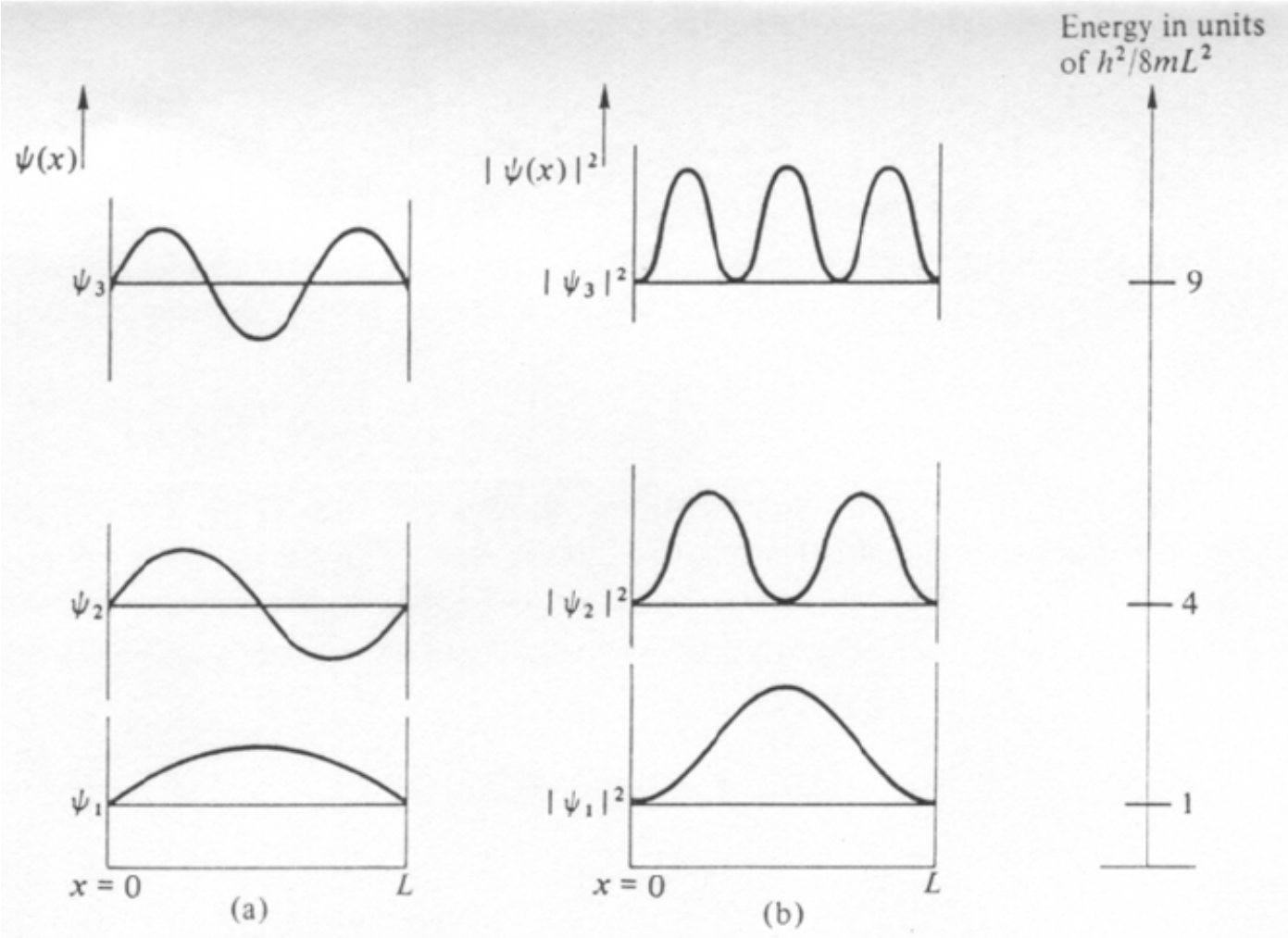
$$k = \sqrt{\frac{2m\ E}{\hbar^2}} \quad \Rightarrow \quad E_n = \frac{n^2h^2}{8mL^2}$$

$$n = -1, -2, \ldots \quad \Rightarrow \quad E_{-n} = E_n$$

k(n,l)

l=1 ↓

l=-1 ↑



$$\Psi_n(x) = C \sin(n\pi x/L)$$

Normovacia podmienka

$$\int_0^L \Psi_n^2 dx = 1 \quad \Rightarrow \quad C = \sqrt{2/L}$$