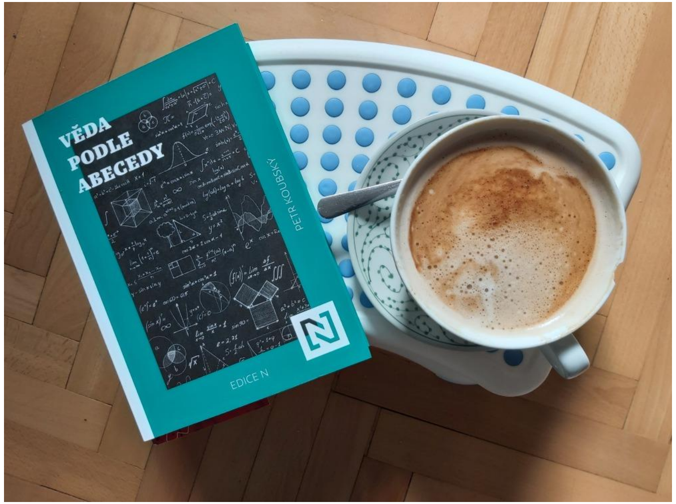

Od Newtona ke Schrödingerovi

aneb

Jak spočítat tvar atomu

PALACKÝ
UNIVERSITY
OLOMOUC

Mgr. Jiří Kvita, Ph.D.
Letní Škola Badatele 2023
Společná laboratoř optiky UP

a photograph of isaac newton sitting in grass under an apple tree with a single red apple falling on his head, with dark sky full of huge planets

Midjourney

Newtonovy zákony

- Newtonovy pohybové zákony
  - Nobelova cena 1687

$$\vec{F} = m \frac{d^2}{dt^2} \vec{x}(t)$$

$$\vec{F} = \frac{d\vec{p}}{dt} = \frac{d}{dt}(m\vec{v})$$

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- A co z nich?
  - Předpověď trajektorie! Lze ověřit, aplikovat.
  - Plynou z nich např. Keplerovy “zákony”.
- Současně: definice síly i hmotnosti.
- Zajímavost: hmotnost setrvačná a gravitační jsou stejné:)

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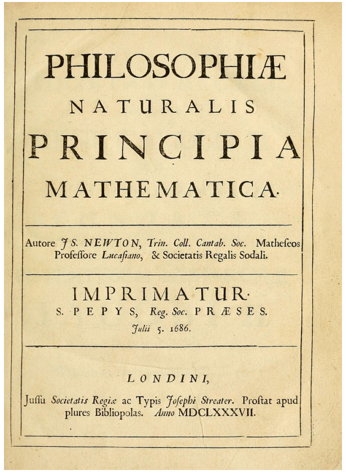
- **Univerzalita gravitace** (jablko, planety)!

$$F_G = \varkappa \frac{m_1 m_2}{|\vec{r}_1 - \vec{r}_2|^2} \qquad V_G = -\varkappa \frac{m_1 m_2}{|\vec{r}_1 - \vec{r}_2|} \qquad \vec{x}(t) = \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix}$$

$$F = -\operatorname{grad} V \qquad F = -\nabla V$$



PHILOSOPHIÆ
NATURALIS
PRINCIPIA
MATHEMATICA.

Autore J S. NEWTON, Trin. Coll. Cantab. Soc. Matheseos Professore Lucasiano, & Societatis Regalis Sodali.

IMPRIMATUR.
S. PEPYS, Reg. Soc. PRÆSES.
Julii 5. 1686.

LONDINI,
Jussu Societatis Regiæ ac Typis Josephi Streater. Prostat apud plures Bibliopolas. Anno MDCLXXXVII.

a photograph of isaac newton sitting in grass under an apple tree with a read apple falling on his head, with dark sky full of huge planets

Midjourney

a photograph of isaac newton sitting in grass under an apple tree with a single red apple falling on his head, with large dark sky with huge planet Saturn on it

Midjourney

red apple falling on the head of isaac newton standing on an asteroid with planet saturn and its rings in the background

Midjourney

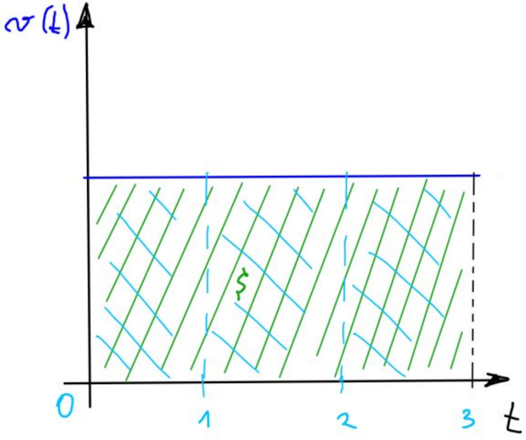
Midjourney

Matematika Newtonových zákonů?

$$\vec{F} = m \frac{d^2}{dt^2} \vec{x}(t)$$

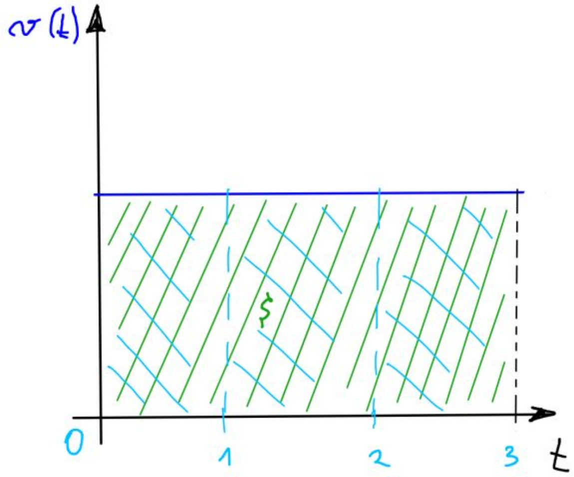
$$\vec{F} = \frac{d\vec{p}}{dt} = \frac{d}{dt}(m\vec{v})$$

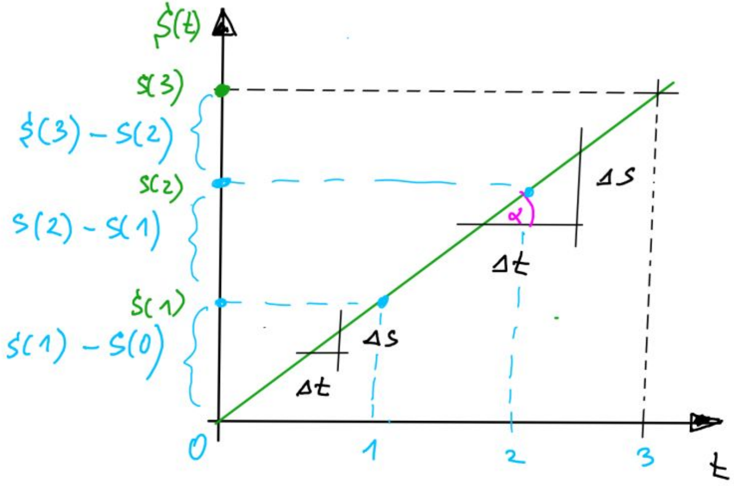
Dráha a rychlost :: rovnoměrný pohyb



$$s = v \cdot t$$

Dráha a rychlost :: rovnoměrný pohyb





$s = v \cdot t$

průměrná $v = \dfrac{\Delta s}{\Delta t} = \mathrm{tg}\,\alpha$

Rovnoměrný pohyb

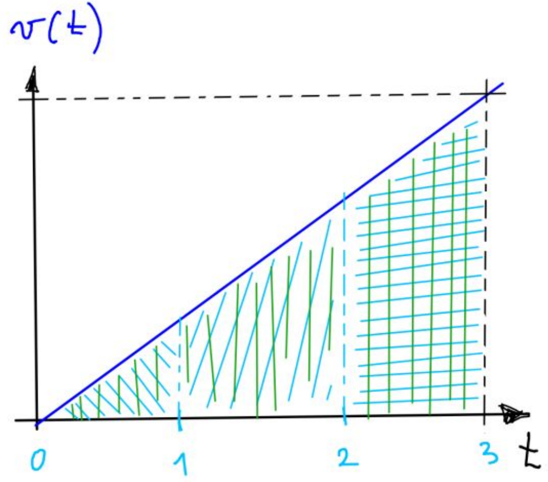
Uražená dráha

Rychlost

okamžitá $v = \dfrac{ds}{dt} \equiv \dot{s}$

přesněji $v(t) = \dfrac{ds(t)}{dt} = \dot{s}(t)$

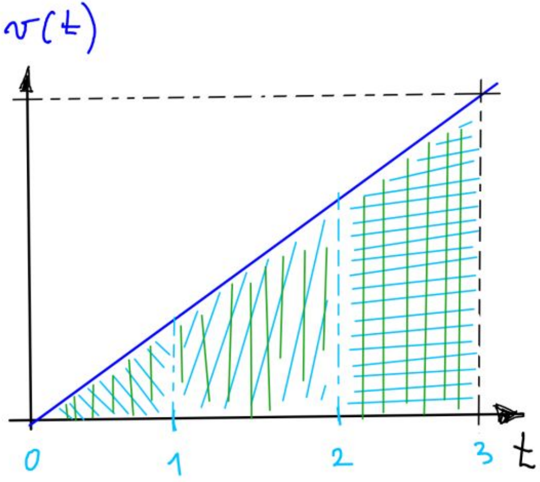
Dráha a rychlost :: volný pád

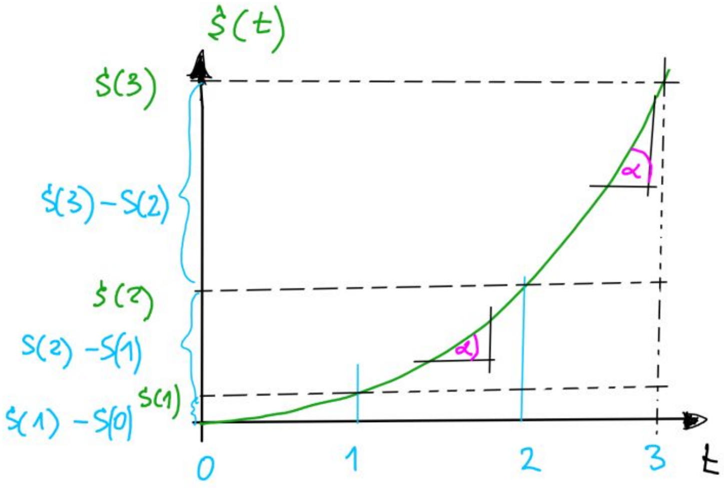


$v = g \cdot t$

Volný pád

Dráha a rychlost :: volný pád





$v = g \cdot t$ Volný pád

$a = \frac{\Delta v}{\Delta t}$ zrychlení

$a(t) = \frac{dv(t)}{dt}$

Celková dráha : plocha

$s = \frac{1}{2} v \cdot t = \frac{1}{2} g \cdot t \cdot t$

$s = \frac{1}{2} g t^2$

$v(t) = \frac{ds(t)}{dt} = \dot{s}(t)$

Rychlost → dráha: Integrace

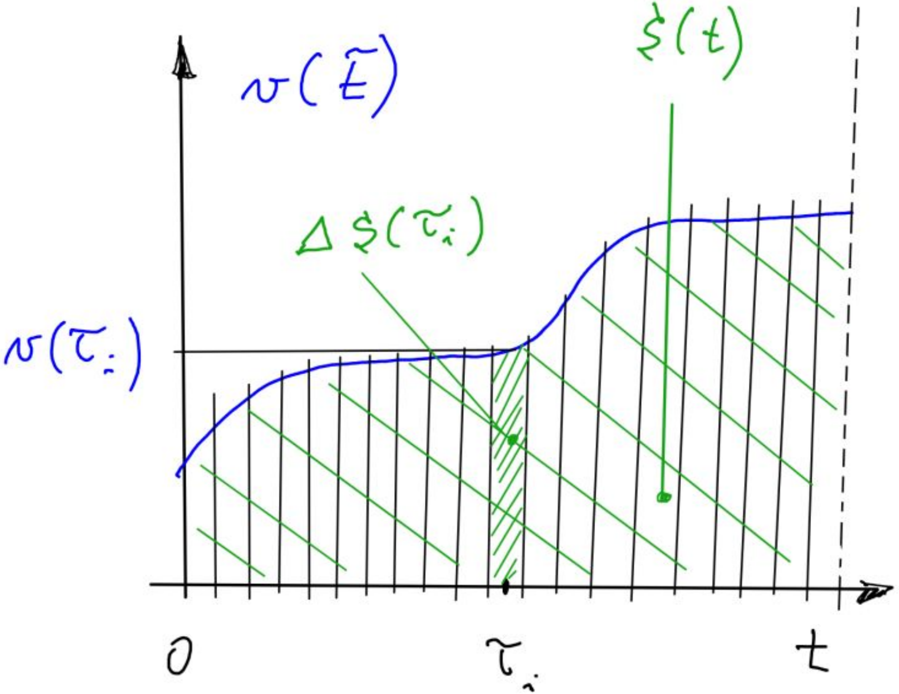
$$\Delta s = v(\tilde{t})\,\Delta\tilde{t}$$

$$\Delta s_i = v(\tilde{t}_i)\,\Delta\tilde{t}$$

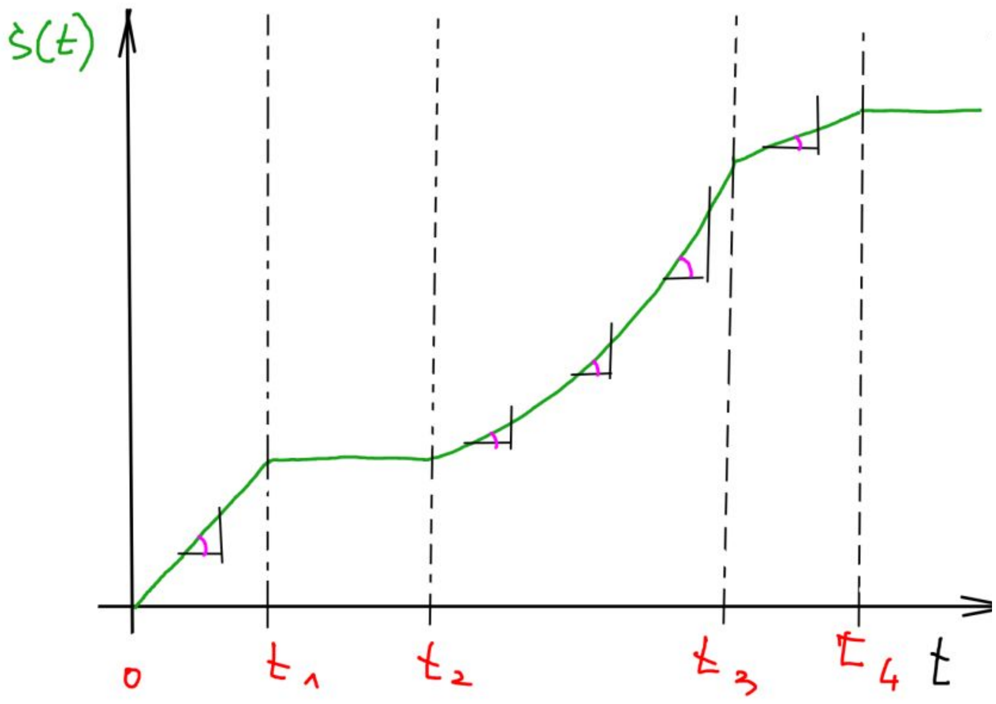
$$s = \sum_i \Delta s_i = \sum_i v(\tilde{t}_i)\,\Delta\tilde{t}_i$$

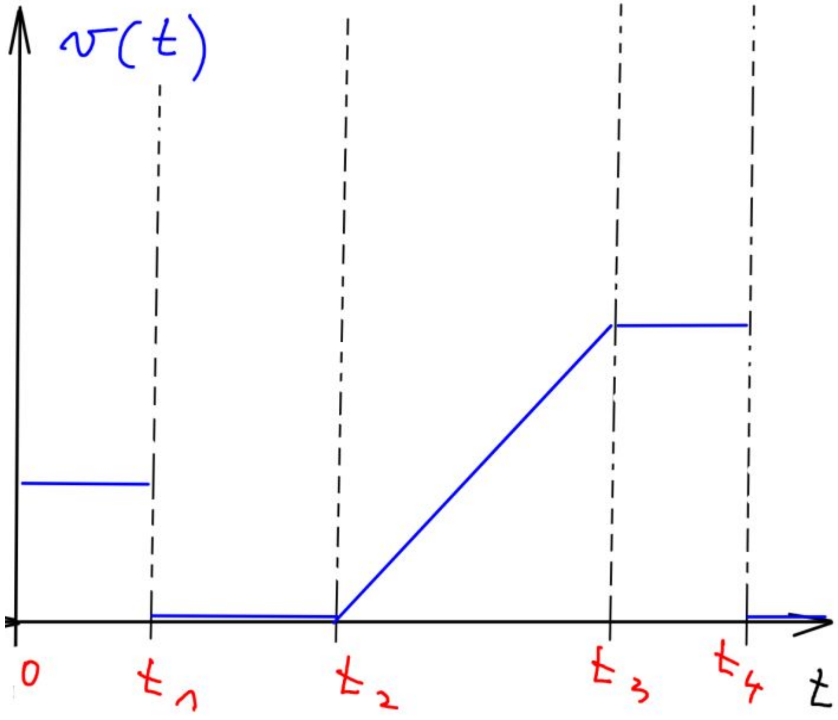
$$ds = v(\tilde{t})\,d\tilde{t}$$

$$s(t) = \int_0^t v(\tilde{t})\,d\tilde{t}$$

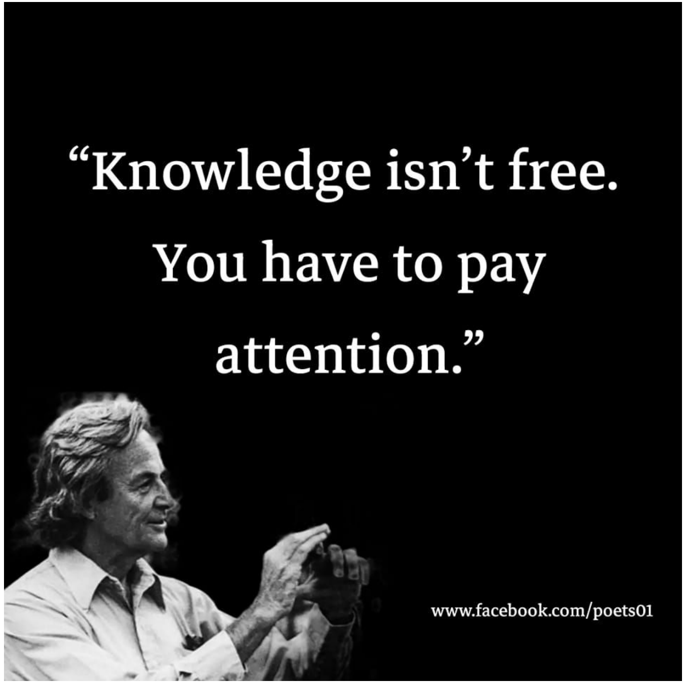


Dráha→ Rychlost: Derivace

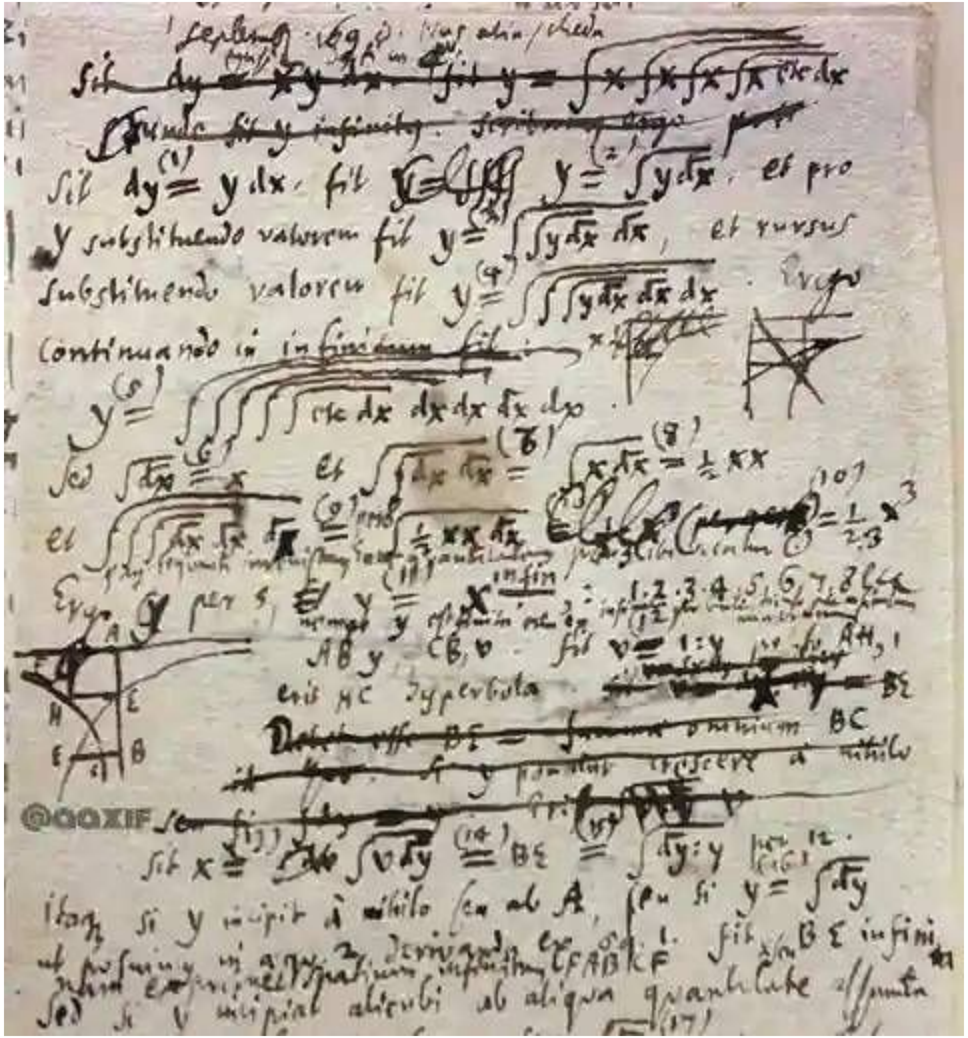




Integrály



Leibnitz

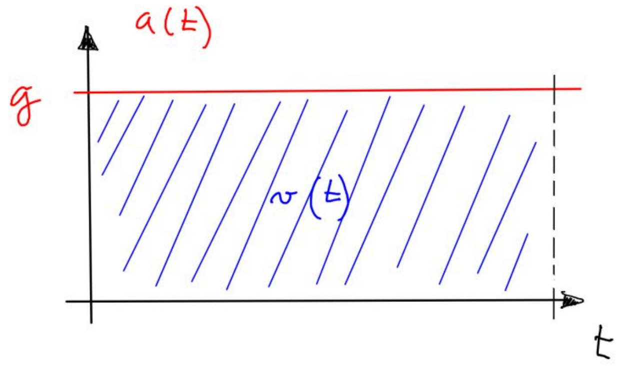


Zrychlení :: volný pád

-

$$a(t) = \dot{v}(t) = \ddot{s}(t)$$

$$a(t) = \frac{dv}{dt} = \frac{d^2 s}{dt^2}$$



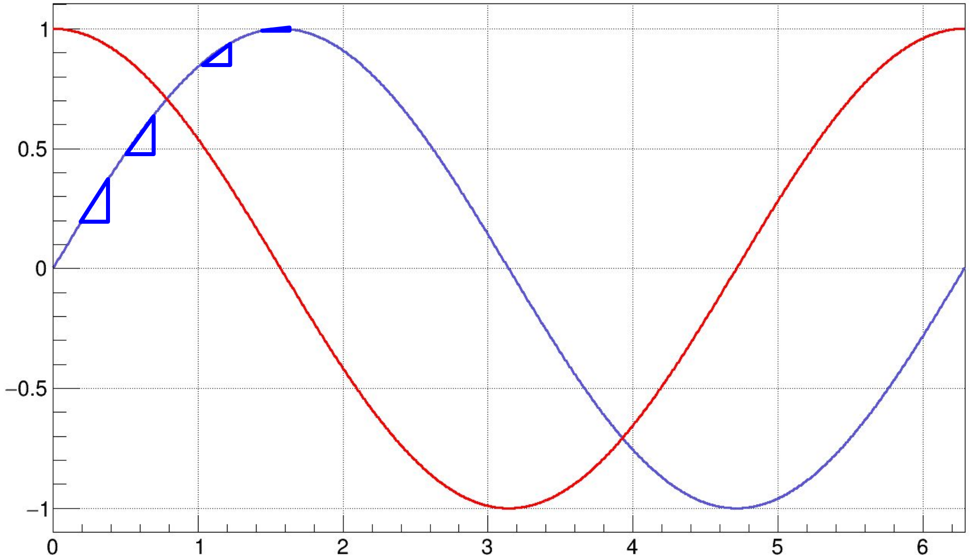
$$v(t) = \int_0^t a(\tilde{t})\, d\tilde{t}$$

$$\vec{F} = m \frac{d^2}{dt^2} \vec{x}(t)$$

$$\vec{F} = \frac{d\vec{p}}{dt} = \frac{d}{dt}(m\vec{v})$$

Sinus a Cosinus

$$\frac{d}{dx} \sin x = \cos x$$

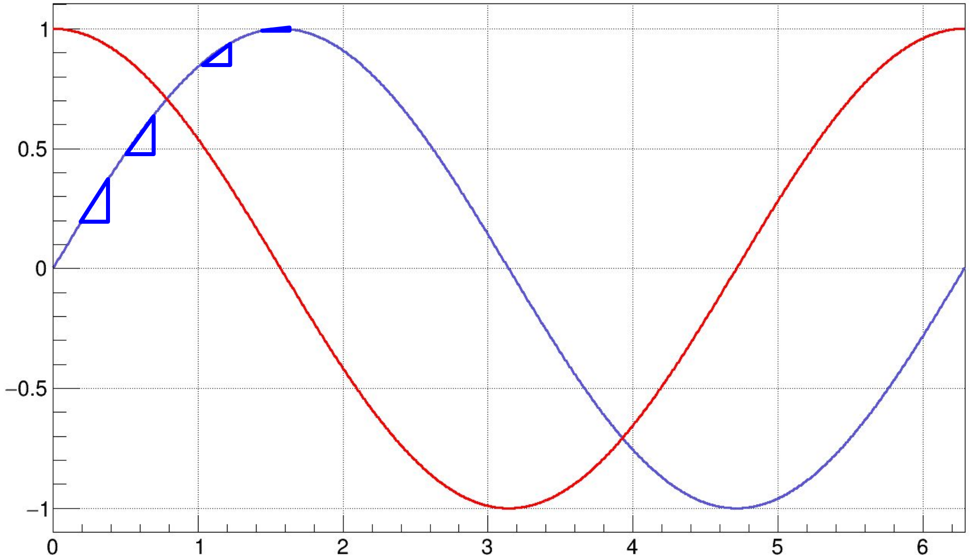


Sinus a Cosinus

- první derivace je rychlost růstu funkce

$$\frac{d}{dx} \sin x = \cos x$$

$$\frac{d}{dx} \cos x = - \sin x$$



Sinus a Cosinus

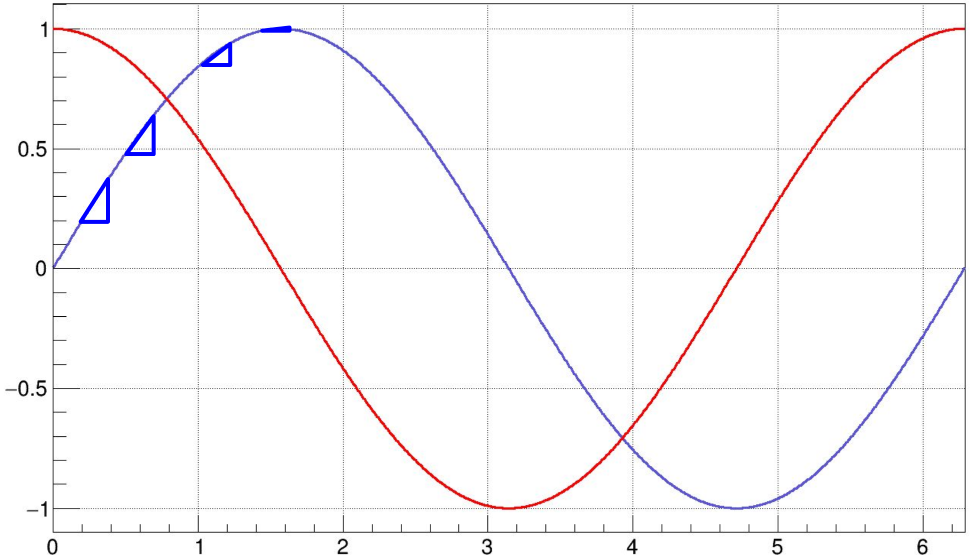
- druhá derivace je křivost funkce

$$\frac{d}{dx} \sin x = \cos x$$

$$\frac{d}{dx} \cos x = - \sin x$$

$$\frac{d^2}{dx^2} \sin x = - \sin x$$

$$\frac{d^2}{dx^2} \cos x = - \cos x$$



Sinus a Cosinus

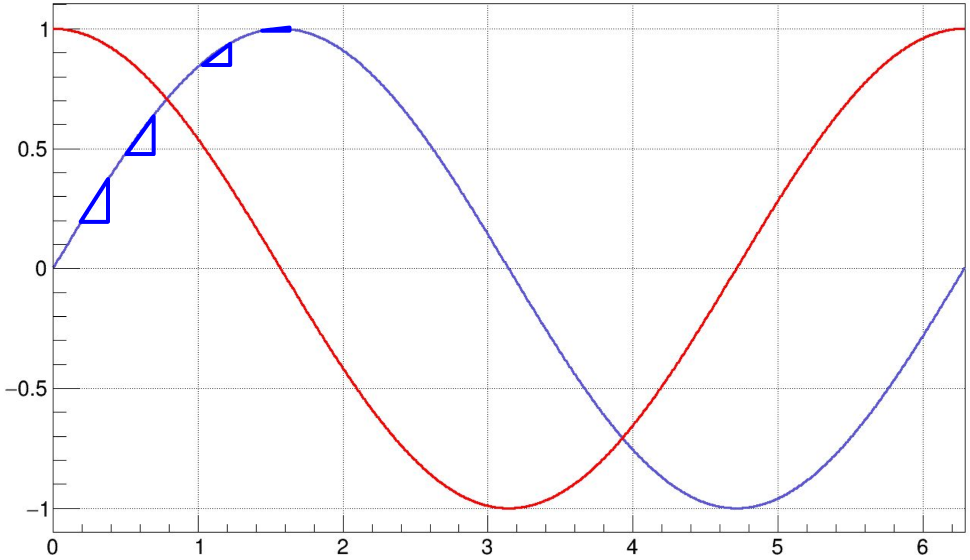
-

$$(\sin x)' = \cos x$$

$$(\cos x)' = -\sin x$$

$$(\sin x)'' = -\sin x$$

$$(\cos x)'' = -\cos x$$



Sinus a Cosinus

$$(\sin kx)' = k \cos kx$$

$$(\cos kx)' = -k \sin kx$$

$$(e^x)' = e^x$$

$$(e^{ax})' = a e^{ax}$$

$$(e^{ikx})' = ik\, e^{ikx} \qquad (e^{ikx})'' = -k^2 e^{ikx}$$

Vlna

- Zobecnění / Povýšení pozorování na princip
- Nechť diferenciální rovnice určuje řešení, kterému budeme říkat vlna

$$\frac{d^2}{dx^2} f(x) = -f(x)$$

$$\Rightarrow \quad f(x) = A \sin x + B \cos x$$

$$f''(x) = -f(x)$$

Vlna

Postupující harmonická vlna

Např. $$f(x,t) = A\cos[k(x - vt)]$$

$$\frac{\partial f}{\partial x} = -kA\sin[k(x - vt)]$$

$$\frac{\partial^2 f}{\partial x^2} = -k^2 A\cos[k(x - vt)] = -k^2 f \quad ! \quad :-)$$

$$\frac{\partial f}{\partial t} = -kvA\sin[k(x - vt)]$$

$$\frac{\partial^2 f}{\partial t^2} = -k^2 v^2 A\cos[k(x - vt)] = -k^2 v^2 f \quad ! \quad :-)$$

Vlnová rovnice

$$1D: \left(\frac{1}{v^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) f(x,t) = 0$$

Vlnová rovnice

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$$1D: \frac{d^2}{dx^2} \qquad 3D: \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \equiv \Delta$$

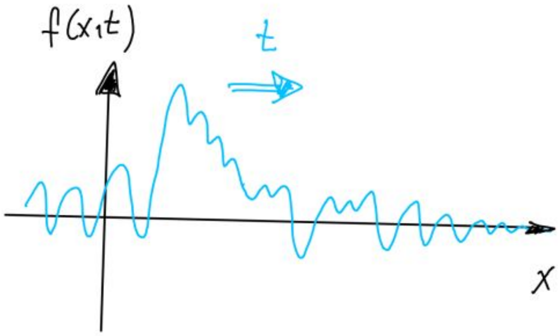
Vlnová rovnice

$$1D: \left(\frac{1}{v^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right) f(x,t) = 0$$

Vlnová rovnice 3D

$$\left(\frac{1}{v^2} \frac{\partial^2}{\partial t^2} - \Delta \right) f(x,t) = 0$$

$$\Box f = 0$$



Posunující se obecná vlna

$$1D: \frac{d^2}{dx^2} \qquad 3D: \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \equiv \Delta$$

Vlnová rovnice

$$1D: \left(\frac{1}{v^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \right) f(x,t) = 0$$

Jean le Rond d'Alembert

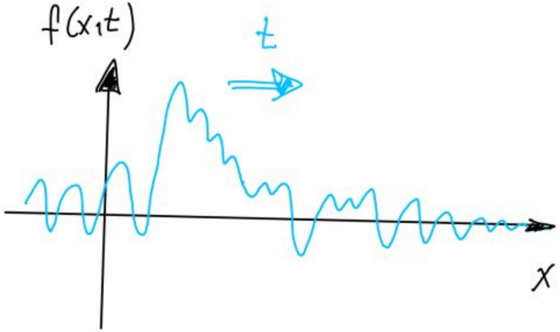
$\Box$

Vlnová rovnice 3D

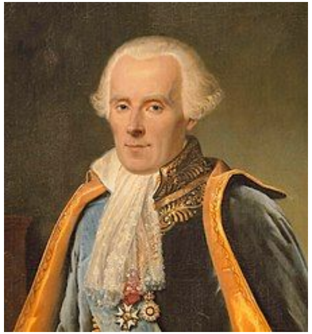
$$\left(\frac{1}{v^2} \frac{\partial^2}{\partial t^2} - \Delta \right) f(x,t) = 0$$

$$\Box f = 0$$

Posunující se obecná vlna



Pierre-Simon Laplace



Δ

$$1D: \quad \frac{d^2}{dx^2} \qquad 3D: \quad \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \equiv \Delta$$

https://www.surfertoday.com/surfing/chicama-the-worlds-longest-wave

Louis de Brogli

- Částice mají i vlnové vlastnosti:
- ⇒ Myšlenka: hmotné vlny
- Částici s hybností má i vlnovou délku:

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

Louis de Broglie

Schrödingerova rovnice

- Ústřední nerelativistická rovnice kvantové mechaniky
- Inspirace vedla k postulátu pohybové rovnice

Erwin Schrödinger

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

$$\Psi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C} \qquad |\Psi|^2 \equiv \Psi\Psi^* = \varrho$$

$$\left[\hat{T} + \hat{V}\right]\Psi = i\hbar\,\partial_t \Psi \qquad \hat{H}\psi = E\psi$$

$$V \neq V(t)$$

Schrödinger

erwin schrodinger with round glasses in light blue suit playing with a pink hairy cat with background of a black board covered with equations

Midjourney

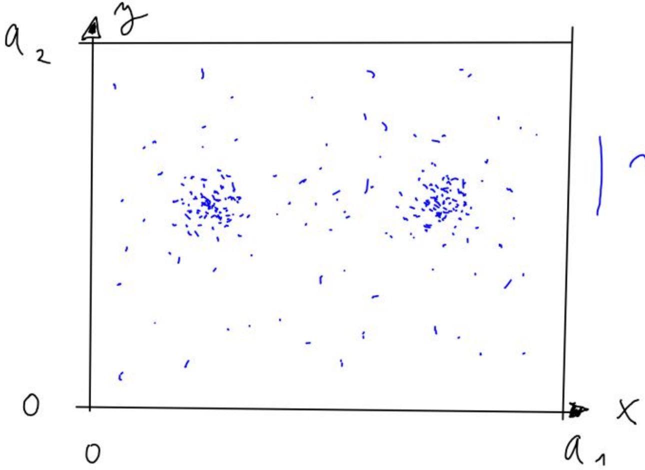
erwin schrodinger with round glasses in light blue suit playing with a pink hairy cat with background of a black board covered with the schrodinger equation

Midjourney

Schrödingerova rovnice: řešení pro částici v krabici

- Vlnová funkce částice je řešením bezčasové Schrödingerovy rovnice pro nulový potenciál, ale částice je omezena na určitou oblast.
- **Řešením jsou stojaté hmotné částicové vlny** a diskrétní možné hodnoty energie: kvantování!

$$\psi_{n_1 n_2}(x,y) \sim \sin\frac{n_1 \pi x}{a_1} \cdot \sin\frac{n_2 \pi y}{a_2}$$



$$\rho \sim |\psi(x,y)|^2$$

$$-\frac{\hbar^2}{2m}\Delta\psi_n = E_n\psi_n$$

+ okr. podm.

$\Rightarrow$ částice v krabici

$\Rightarrow$ stojaté vlny

$$E_n = \frac{(n\pi\hbar)^2}{2ma^2} = \frac{(n\pi)^2(\hbar c)^2}{2mc^2\, a^2}$$

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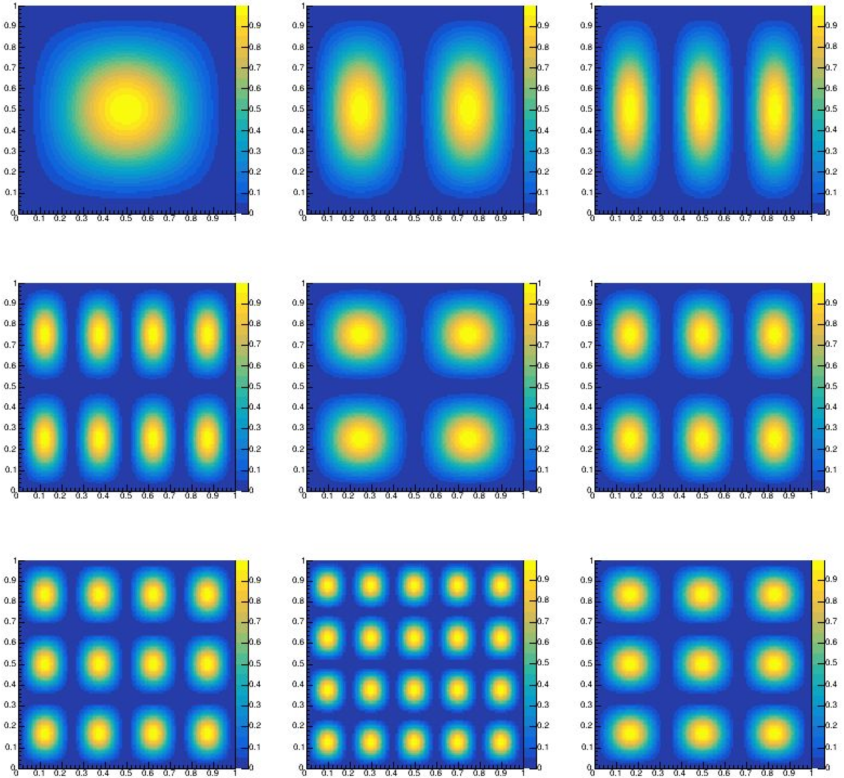

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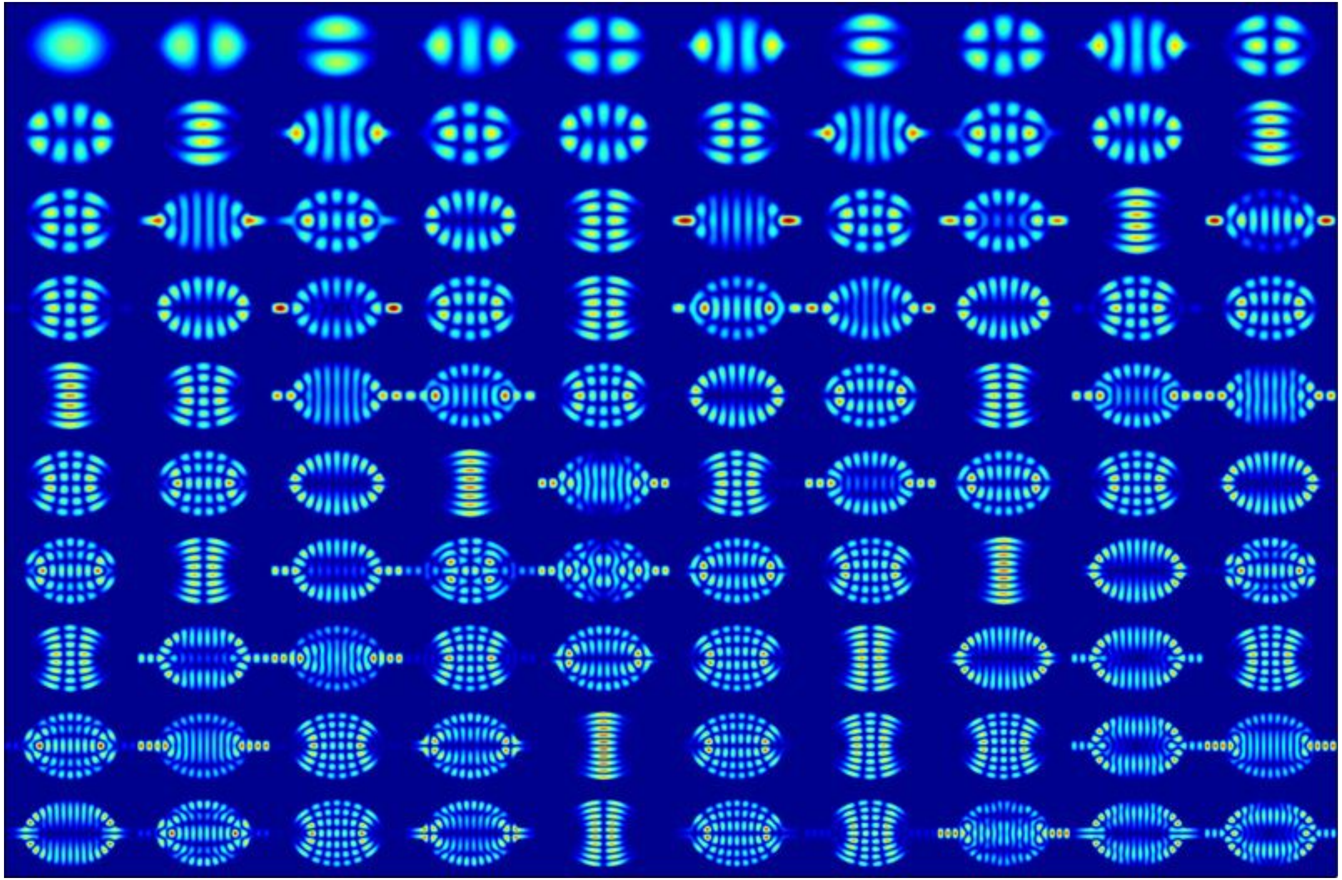
Částice v krabici

- Kvantový billiard na elipse



Atom vodíku

- Bohrův model atomu
- Vycházel z heuristického kvantování momentu hybnosti
- Rozměr Planckovy konstanty h je rozměr momentu hybnosti:)
- Vedlo na kvantování energie elektronu v atomu a na vysvětlení spekter atomů.
- Ale nešlo zobecnit na další systémy.

Niels Bohr

$$L_n \equiv n\hbar \qquad p = \frac{h}{\lambda}$$

$$E = E_p + E_k$$

$$p_n = \frac{h}{\lambda_n} \qquad L_n = r_n p_n$$

Atom vodíku

- Vlnová funkce elektronu je řešením bezčasové Schrödingerovy rovnice pro Coulombický potenciál.
- Možná matematicky pěkná a fyzikální řešení jsou velmi specifická.
- Jdou ruku v ruce s omezenými a diskrétními možnými hodnotami energie: kvantování!

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

$$V = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r} \qquad V = -\frac{\alpha\hbar c}{r}$$

$$\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \doteq \frac{1}{137}$$

$$\hbar c \doteq 197\ \mathrm{MeV}\cdot\mathrm{fm}$$

Atom vodíku

- Řešit zvlášť rovnice jako funkce poloměru a úhlů
- Vyřešit kvantování momentu hybnosti.

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \varphi^2}$$

$$\Delta = \Delta_r - \frac{1}{r^2}\frac{\hat{L}^2}{\hbar}$$

$$L^2 Y_l^m(\theta, \varphi) = \hbar^2 l(l+1) Y_l^m(\theta, \varphi)$$

$$L_z Y_l^m = m\hbar Y_l^m$$

$$Y_l^m = L_l^{|m|}(\cos\theta)\, e^{im\varphi}$$

Atom vodíku – poznámky k momentu hybnosti

		#	+ spin x 2	
$\ell = 0$	... s	1	2	
$\ell = 1$	... p	3	6	$2\ell + 1$
$\ell = 2$	... d	5	10	$m = -\ell, \dots, \ell$
$\ell = 3$	... f	7	14	

$$E_n \longmapsto E_{n,\ell}$$

1s 2s 2p 3s 3p 4s 3d

Atom vodíku

- Rovnice nesoucí závislost na poloměru se podobá 1D Sch. rovnici a vede na kvantování energií.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\,\psi(x) \qquad \dots 1D$$

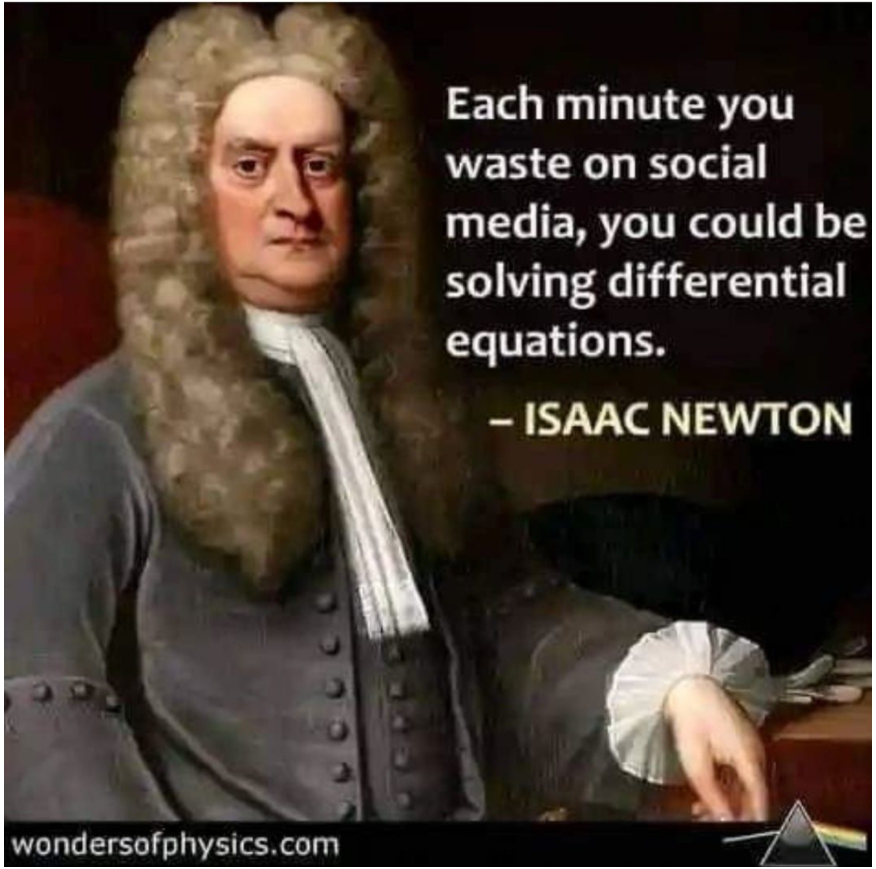
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u(r) = E\,u(r)$$

$$u(r) = \frac{R(r)}{r}$$

$$\psi(r,\theta,\varphi) \equiv R(r)\,Y(\theta,\varphi)$$

$$\psi_{nlm}(r,\theta,\varphi) \equiv R_{nl}(r)\,Y_l^m(\theta,\varphi)$$

A gentle reminder…

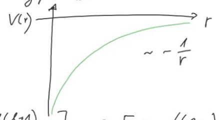


Atom vodíku

23.11.2020 KM 1

– aprox. případ centrálního pole; Coulombický potenciál:

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$$



Dovolené E v QM pro $V(r)$

⇒ řešíme radiální rovnici pro $V(r)$

$$-\frac{\hbar^2}{2m}u'' + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \quad \Big/ \cdot\left(\frac{2m}{\hbar^2}\right)$$

$u(r)$, $R = \frac{u}{r}$!

Řešíme vázané stavy: $E < 0$

$$-\frac{2mE}{\hbar^2} \equiv \varkappa^2$$

$[\varkappa] = [r]^{-1} \Rightarrow \rho \equiv \varkappa r \quad \rho$ … bezrozměrné

1

$$u'' + \frac{2m}{\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{u}{r} - \left[\frac{l(l+1)}{r^2} + \varkappa^2\right]u = 0 \quad \Big/ \frac{1}{\varkappa^2}$$

$$\hbar c \cdot \frac{e^2}{4\pi\varepsilon_0 \hbar c} \equiv \alpha$$

$$\frac{1}{\varkappa^2}u'' + \frac{2mc}{\hbar\varkappa^2}\alpha\frac{u}{r} - \left[\frac{l(l+1)}{\varkappa^2 r^2} + 1\right]u = 0$$

$$\boxed{\frac{2mc}{\hbar\varkappa}\alpha} \boxed{\frac{u}{\varkappa r}}, \quad \frac{2mc}{\hbar\varkappa}\alpha = \rho_0, \quad \varkappa r = \rho, \quad \varkappa^2 r^2 = \rho^2, \quad \rho \equiv \varkappa r$$

$$r = \frac{\rho}{\varkappa} \Rightarrow dr = \frac{1}{\varkappa}d\rho, \quad \frac{1}{dr} = \varkappa\frac{1}{d\rho}$$

$u = u(r) \equiv u(r(\rho))$

$$u' = \frac{du}{dr}; \quad \frac{d}{d\rho}u(r(\rho)) = \frac{du}{dr}\frac{dr}{d\rho} = \frac{1}{\varkappa}\frac{du}{dr} = \frac{1}{\varkappa}u'$$

$$\Rightarrow u' = \varkappa\frac{d}{d\rho} \Rightarrow u'' = \varkappa^2\left(\frac{d}{d\rho}\right)^2$$

2

$v(\rho) \equiv u(r(\rho))$

$$v'' + \frac{\rho_0}{\rho}v - \left(\frac{l(l+1)}{\rho^2} + 1\right)v = 0$$

$\rho \in (0, \infty)$.

Hledáme asymptotické řešení: $\rho \to 0$; $\rho \to \infty$ … chceme kvadraticky integrovatelné fce.

v ODR: $\sim\frac{1}{\rho}$, $\sim\frac{1}{\rho^2}$!

$v \underset{\rho\to\infty}{\to} 0$

1) $\rho \to \infty$: ODR ≃ $v'' \approx v \Rightarrow v(\rho) = \cancel{A e^{\rho}} + B e^{-\rho}$

zamítneme divergentní

$v \sim e^{-\rho}$

3

2) $\rho \to 0$: $v'' \approx \frac{l(l+1)}{\rho^2}v$.

Zkusme: $v \sim \rho^{l+1}$: $v' = (l+1)\rho^l \sim \frac{l+1}{\rho}v$

$v'' = l(l+1)\rho^{l-1} \sim \frac{l(l+1)}{\rho^2}v$

nebo: $v \sim \rho^{-l}$: $v' \sim -l\rho^{-l-1} \sim -l\frac{v}{\rho}$

$v'' \sim (-l)(-l-1)\rho^{-l-2} \sim l(l+1)\frac{v}{\rho^2}$

obec. $\rho \to 0$: $v(\rho) = C\rho^{l+1} + \cancel{D\rho^{-l}}$

ale: $l = 0, 1, \ldots$ ⟶ zamítneme :-)

$R \sim \frac{u}{r}$

4

Celk. asympt. řeš.: $v(\rho) \sim e^{-\rho}\rho^{l+1}$

Zkusme hledat přesné řeš. ve tvaru: $v(\rho) \equiv \rho^{l+1}e^{-\rho}w(\rho)$ (♡)

kde $w(\rho)$ je polynom: $w(\rho) \equiv \sum_{j=0}^{\infty} c_j \rho^j \quad c_j \in \mathbb{C}/\mathbb{R}$

Nutno dosadit nálsadu do radiální rce $v(\rho)$;

dostaneme rci pro $w(\rho)$; hledáme c_j.

Nárok: budeme chtít konečný stupeň polynomu ⇒ kvantování!

n.b.:

$$v'' = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]v$$

Nutné: v' dle (♡)

v'' –"–:

5

$$v \equiv e^{-\rho}\rho^{l+1}w$$

$$v' = e^{-\rho}\left[-\rho^{l+1}w + (l+1)\rho^l w + \rho^{l+1}w'\right] =$$

$$= e^{-\rho}\rho^l\left[(l+1-\rho)w + \rho w'\right]$$

$$v'' = l\rho^{l-1}e^{-\rho}[\ldots] - \rho^l e^{-\rho}[\ldots] + \rho^l e^{-\rho}\left[-w + (l+1-\rho)w' + w' + \rho w''\right] =$$

$$= e^{-\rho}\rho^{l-1}\Big\{(l-\rho)\left[(l+1-\rho)w + \rho w'\right] - \rho w + (l+1-\rho)\rho w' + \rho w' + \rho^2 w''\Big\} =$$

$$= e^{-\rho}\rho^l\left[\left(\frac{l+1-\rho}{\rho}(l-\rho) - 1\right)w + w'\Big[\underbrace{l-\rho+l+1-\rho+1}_{2l-2\rho+2}\Big] + \rho w''\right]$$

$$\frac{l(l+1)}{\rho} - l - l - 1 + \rho - 1 = \left(\frac{l(l+1)}{\rho} - 2l - 2 + \rho\right)$$

6

Máme: $v'' = \rho^l e^{-\rho}\left[\left(\frac{l(l+1)}{\rho} - 2l - 2 + \rho\right)w + 2(l-\rho+1)w' + \rho w''\right]$

Nyní: Dosadit do: $v'' = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] \cdot v$, $\boxed{v = e^{-\rho}\rho^{l+1}w}$

⇒ Rce pro polynom w:

+ zkrátíme $e^{-\rho}$; zkrátíme ρ^l ⇒

$$\left(\cancel{\frac{l(l+1)}{\rho}} - 2l - 2 + \rho\right)w + 2(l-\rho+1)w' + \rho w'' = \left[1 - \frac{\rho_0}{\rho} + \cancel{\frac{l(l+1)}{\rho^2}}\right]\rho w \quad \Big/ \frac{1}{\rho}$$

$$w'' + 2\frac{l-\rho+1}{\rho}w' + \left[\frac{-2l-2+\cancel{\rho}}{\rho} - \cancel{1} + \frac{\rho_0}{\rho}\right]w = 0$$

$$\boxed{w'' + 2\frac{l+1-\rho}{\rho}w' + \left(\frac{\rho_0}{\rho} - 2\frac{l+1}{\rho}\right)w = 0} \quad (*)$$

7

Nyní: $w = \sum_{j=0}^{\infty} c_j\rho^j$ ① pro zájemce :-)

$$w' = \sum_{j=0}^{\infty} j c_j \rho^{j-1} = \sum_{j=0}^{\infty} c_{j+1}(j+1)\rho^j$$ ②

↳ 1. člen je nula; $j \mapsto j+1$; pozn. $\sum_{j=0} \mapsto \sum_{j=1} \mapsto \sum_k$, $k = j-1$, $k \to j$

$$w'' = \sum_{j=1}^{\infty} c_j j(j-1)\rho^{j-2} = \sum_{j=0} c_{j+1}(j+1)\cdot j\rho^{j-1}$$ ③

$k = j-1$, $k \to j$

Motivace: v ODR pro w budeme chtít srovnat koef. u stejné mocniny ρ + suma $\sum_{j=0}$!

Dosadíme do (*)

$$\sum_{j=0}^{\infty}\Big\{\underbrace{c_{j+1}j(j+1)\rho^{j-1}}_{③,\ \text{člen} \sim w''} + 2(l+1)c_{j+1}(j+1)\rho^{j-1} - 2c_j\rho^{j-1}\cdot j +$$

① člen u $w' \sim \frac{2(l+1)}{\rho}$; ② člen u $w' \sim \frac{-\rho}{\rho}$

8

$$+ \rho_0 c_j \frac{\rho^{j-1}}{\cancel{\rho}} - 2(l+1)c_j\rho^{j-1}\Big\} = 0$$

$$\Rightarrow \sum_{j=0}^{\infty}\rho^{j-1}\Big\{\ \ldots\ \Big\} = 0$$

srovnání koef. ρ^{j-1}

$$c_{j+1}j(j+1) + 2(l+1)c_{j+1}(j+1) - 2jc_j + \rho_0 c_j - 2(l+1)c_j = 0$$

$$c_{j+1} = \frac{2(l+1+j) - \rho_0}{(j+1)(j+2l+2)}c_j$$

… rekurzivní vztah pro c_{j+1} = fce c_j

Asympt. $j \to \infty$: $c_{j+1} \approx \frac{2\cancel{j}}{(j+\cancel{1})\cdot \cancel{j}}c_j$

9

Asympt.: $j \to \infty$, tj. velké mocniny ρ v rozvoji $w = \sum c_j\rho^j$:

$$c_{j+1} \simeq c_j\frac{2}{j} \Rightarrow c_j \simeq c_0\frac{2^j}{j!}$$

Ale: $w \simeq c_0\sum\frac{2^j\rho^j}{j!} = c_0\sum\frac{(2\rho)^j}{j!} = c_0\boxed{e^{2\rho}}$

Ale: $v(\rho) = \boxed{e^{-\rho}}\rho^{l+1}\cdot w$

pokazí asympt. chování a řešení vede divergentní pro $\rho \to \infty$ ⇒

⇒ Potřebujeme, aby w byl polynom konečného stupně!

$$\exists\, j_{max}: \quad c_{j_{max}+1} = 0$$

10

$$c_{j+1} = c_j\frac{2(l+j+1) - \rho_0}{(j+1)(j+2l+2)} \quad \longrightarrow$$

$c_{j_{max}+1} = 0$; $c_j \neq 0$

$$2(\underbrace{l + j_{max} + 1}_{\equiv n}) - \rho_0 = 0$$

$l = 0, 1, \ldots$; $j_{max} = 0, 1, \ldots$ ⇒ $n = 1, 2, \ldots$, $n \in \mathbb{N}$

n.b.: $\rho_0 = \frac{2mc}{\hbar\varkappa}\alpha \ \wedge\ 2n = \rho_0$ … z ukončení polynomu

ale: $\varkappa^2 = -\frac{2mE}{\hbar^2}$! ⇒ $4n^2 = \rho_0^2$

11

$2n = \rho_0 \quad / ()^2$

$$4n^2 = \rho_0^2 = \left(\frac{2mc}{\hbar\varkappa}\right)^2\alpha^2 \qquad \varkappa^2 = \boxed{-\frac{2mE}{\hbar^2}}$$

$$\cancel{4}n^2 = \frac{\cancel{4}m^{\cancel{2}}c^2}{\cancel{\hbar^2}}\alpha^2\cdot\boxed{-\frac{\cancel{\hbar^2}}{2mE}}$$

$$\boxed{E_n = -\frac{1}{2}\frac{mc^2}{n^2}\cdot\alpha^2}$$

→ velmi důležitý výsledek QM ! ✓ :-)

… energetické hladiny elektronu ($m \equiv m_e$:-)

v Coulombickém potenciálu (aproximace ∞ těžkého jádra),

zde dle principů QM, tj. hledání spektra $\hat{H}$: $H\psi = E\psi$

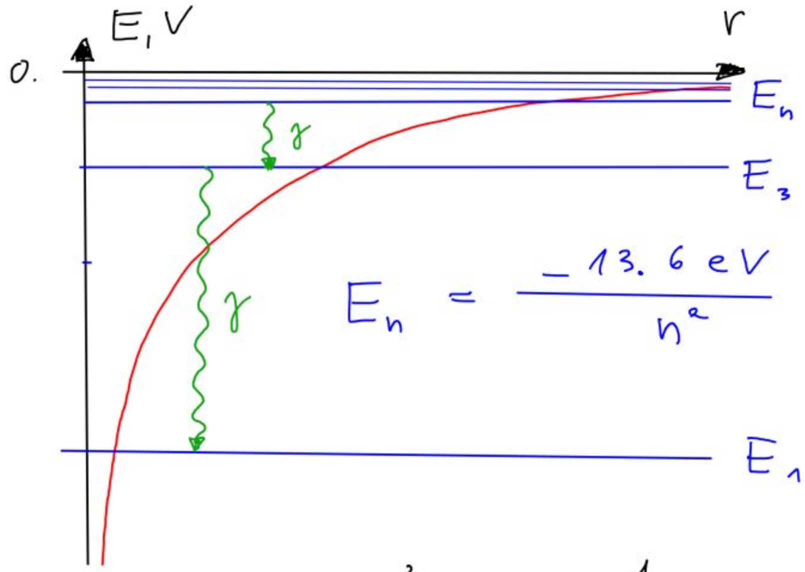
a za požadavku kvadrat. integrovatelného řešení! :-)

– shodné s Bohrovým poloklas. odvoz. vztahem :-)

12

Atom vodíku

- Schr. rovnice řešitelná jen pro určité energie: kvantování!
- Vysvětlení diskrétních spekter atomů a molekul! – přechody mezi hladinami.



$$V(r) \sim \frac{-e^2}{r}$$

$$E_n = \frac{-13.6\ \mathrm{eV}}{n^2}$$

vázaný stav

$$E = E_k + E_p < 0$$

$$E_\gamma = E_m - E_n = \frac{13.6\ \mathrm{eV}}{n^2 - m^2}$$

$$\alpha \equiv \frac{e^2}{4\pi\varepsilon_0 \hbar c} \doteq \frac{1}{137}$$

$$E_n = -\frac{1}{n^2}\,\frac{1}{2}\,\alpha^2\, m_e c^2 \qquad m_e c^2 \doteq 511\ \mathrm{keV}$$

Atom vodíku

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

$$\psi(\vec{x}) \equiv \psi_{n\ell m}(\vec{x}) = R_{n\ell}(r)\,Y_{\ell m}(\vartheta, \varphi)$$

$$\equiv \psi_{n\ell m}(r, \vartheta, \varphi)$$

- Určitým energiím přísluší určité vlnové funkce.
- Ale k čemu je vlnová funkce?

Atom vodíku

- Určitým energiím přísluší určité vlnové funkce.
- Ale k čemu je vlnová funkce?
- Vlnová funkce ⇒ pravděpodobnost, s jakou elektron nalezneme okolo jádra.

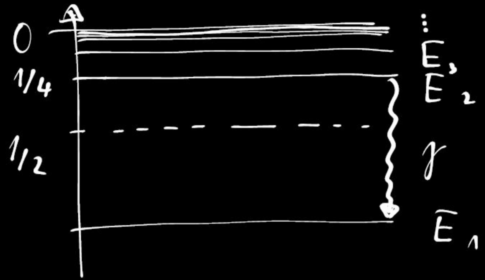
Max Born

$$\psi = \psi(x, y, z) = \psi(r, \theta, \varphi)$$

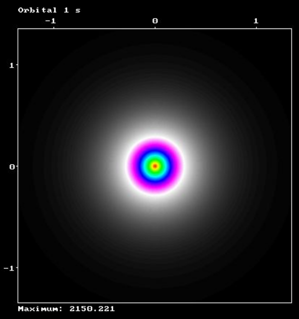
$$\varrho(\vec{x}) = |\psi(\vec{x})|^2$$ hustota pravděpodobnosti

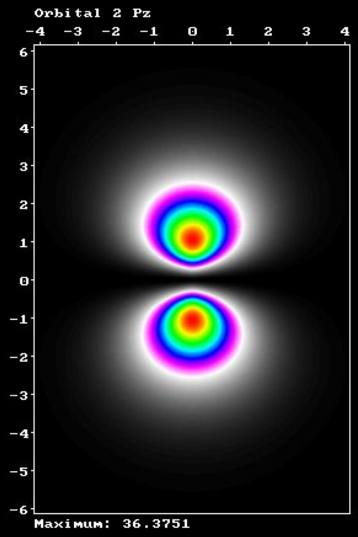
Atom vodíku

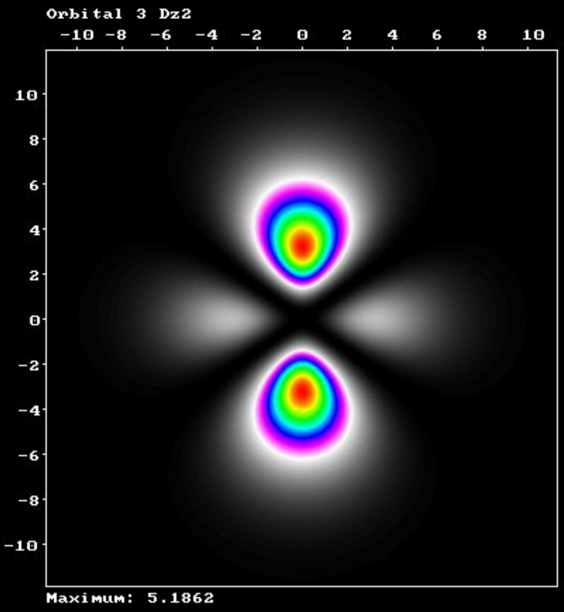
- Různé pravděpodobnosti nalezení elektronu okolo jádra
  - pro různé energie, hodnoty dalších kvantových čísel
  - jde o různé vlnové funkce, tj. stavy elektronu v atomu.
  - Elektron je stojatá částicová vlna okolo jádra.
  - Mikrosvět a kvantová mechanika jsou pravděpodobnostní!
  - Albert Einstein: Bůh nehraje v kostky!



$$E_n = -\frac{13.6\,eV}{n^2}$$



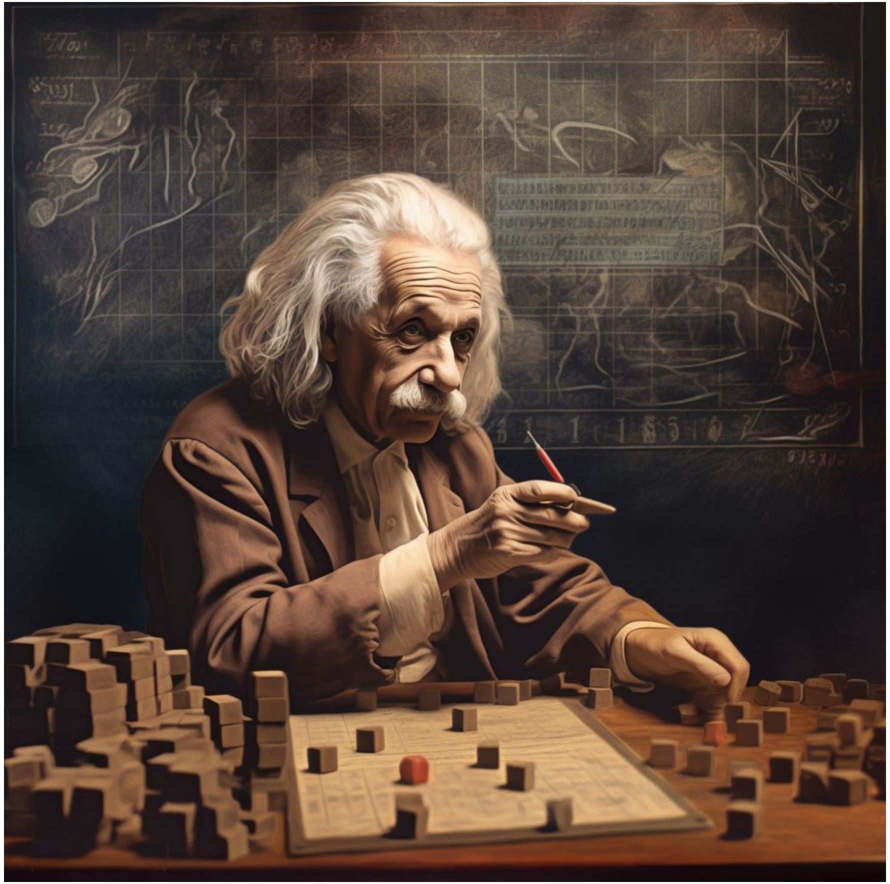




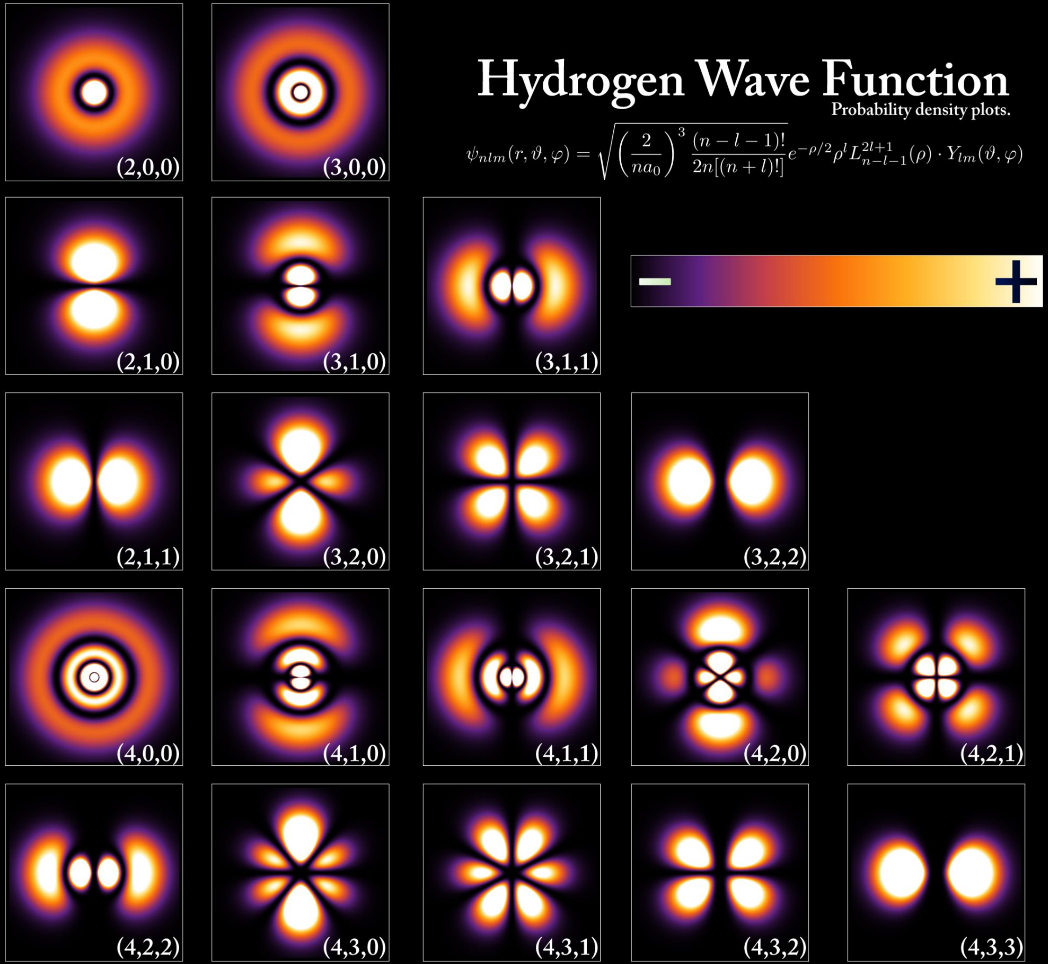
“Bůh nehraje v kostky”, Albert Einstein

Midjourney

Albert Einstein playing dice with the God at a table with background of black boards covered with equations



https://en.wikipedia.org/wiki/Atomic_orbital



$$1s = \frac{1}{\pi^{1/2}}\left(\frac{Z}{a}\right)^{3/2} e^{-Zr/a}$$

$$2s = \frac{1}{4(2\pi)^{1/2}}\left(\frac{Z}{a}\right)^{3/2}\left(2 - \frac{Zr}{a}\right)e^{-Zr/2a}$$

$$2p_z = \frac{1}{4(2\pi)^{1/2}}\left(\frac{Z}{a}\right)^{5/2} re^{-Zr/2a} \cos\theta$$

$$2p_x = \frac{1}{4(2\pi)^{1/2}}\left(\frac{Z}{a}\right)^{5/2} re^{-Zr/2a} \sin\theta \cos\phi$$

$$2p_y = \frac{1}{4(2\pi)^{1/2}}\left(\frac{Z}{a}\right)^{5/2} re^{-Zr/2a} \sin\theta \sin\phi$$

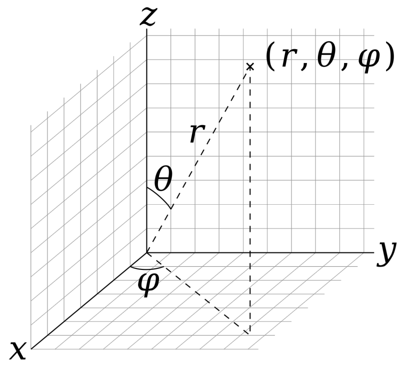
$$3s = \frac{1}{81(3\pi)^{1/2}}\left(\frac{Z}{a}\right)^{3/2}\left(27 - 18\frac{Zr}{a} + 2\frac{Z^2r^2}{a^2}\right)e^{-Zr/3a}$$

$$3p_z = \frac{2^{1/2}}{81\pi^{1/2}}\left(\frac{Z}{a}\right)^{5/2}\left(6 - \frac{Zr}{a}\right)re^{-Zr/3a} \cos\theta$$

$$3p_x = \frac{2^{1/2}}{81\pi^{1/2}}\left(\frac{Z}{a}\right)^{5/2}\left(6 - \frac{Zr}{a}\right)re^{-Zr/3a} \sin\theta \cos\phi$$

$$3p_y = \frac{2^{1/2}}{81\pi^{1/2}}\left(\frac{Z}{a}\right)^{5/2}\left(6 - \frac{Zr}{a}\right)re^{-Zr/3a} \sin\theta \sin\phi$$

$$3d_{z^2} = \frac{1}{81(6\pi)^{1/2}}\left(\frac{Z}{a}\right)^{7/2} r^2e^{-Zr/3a}(3\cos^2\theta - 1)$$



https://en.wikipedia.org/wiki/Spherical_coordinate_system

https://www.pearsonhighered.com/assets/samplechapter/0/3/2/1/0321803450.pdf

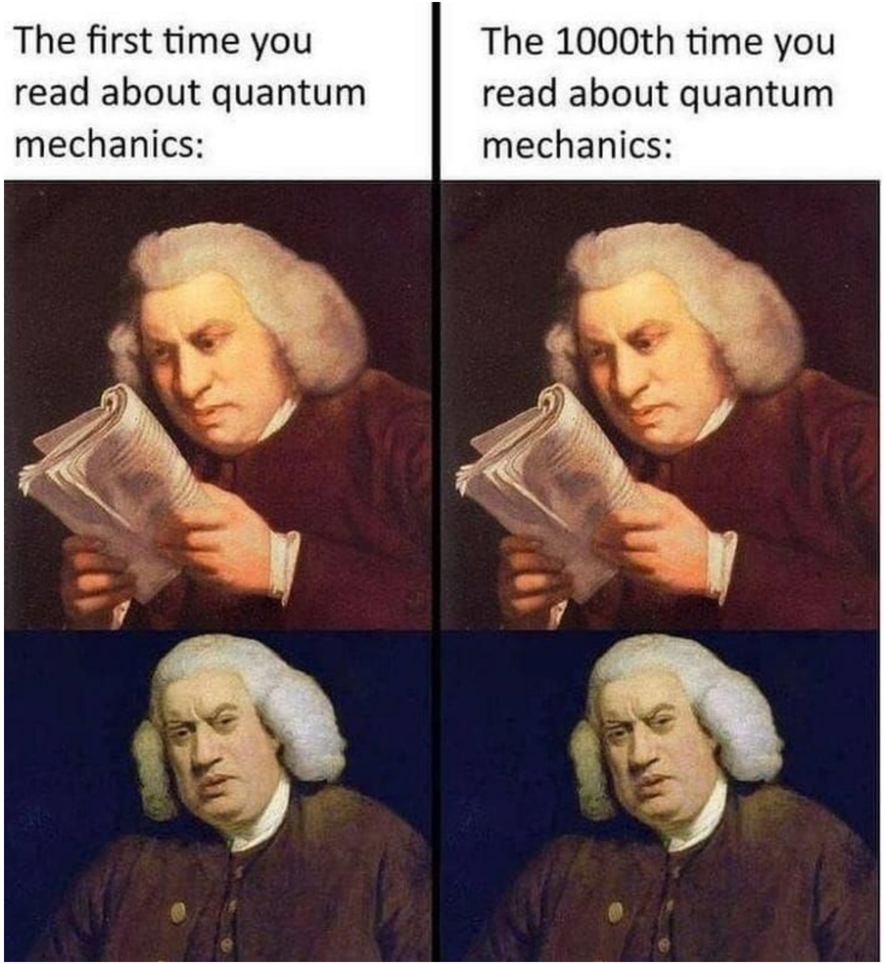
Závěr I

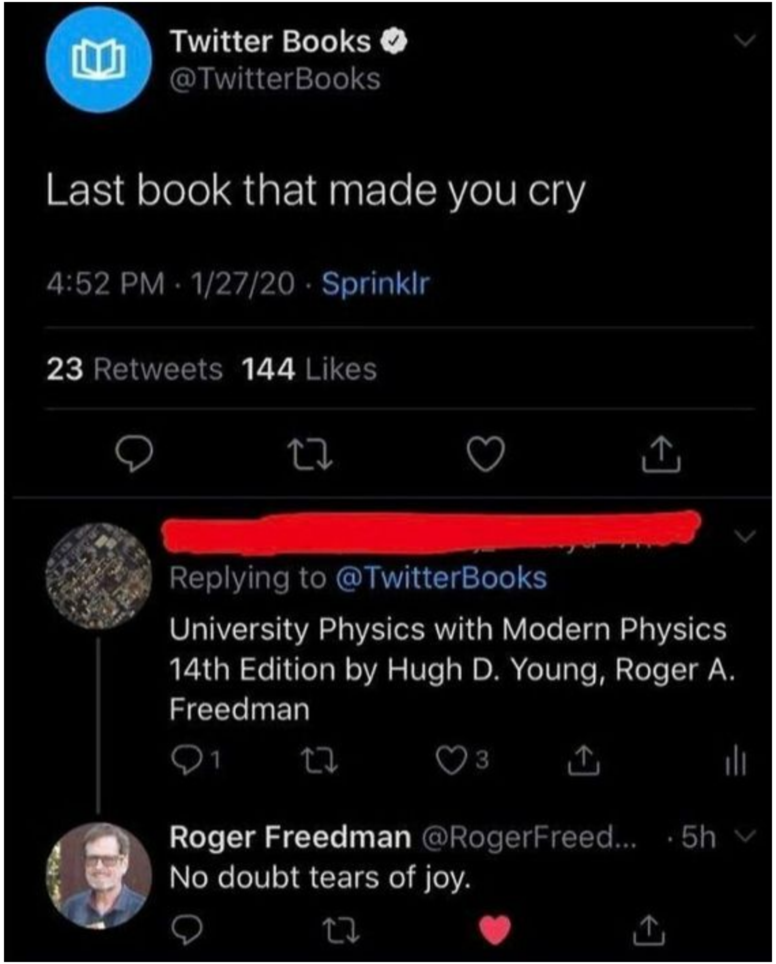
$$\vec{F} = m \frac{d^2}{dt^2} \vec{x}(t)$$

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

Závěr II

PYTHAGOREAN THEOREM
(GEOMETRY)
$a^2 + b^2 = c^2$
This theorem, proposed by ancient Greek mathematician Pythagoras, relates the lengths of the sides of a right-angled triangle. It is a fundamental principle in Euclidean geometry and has been used extensively in various fields, including physics, computer graphics, and engineering design.
FOURIER TRANSFORM
(SIGNAL PROCESSING)
$F(\omega) = \int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt$
Developed by Joseph Fourier in the early 19th century, the Fourier Transform allows a mathematical function to be decomposed into its constituent frequencies. This technique is fundamental in the field of signal processing and has found applications in areas like image processing, audio signal processing, and solving partial differential equations.
EINSTEIN'S EQUATION
(SPECIAL RELATIVITY)
$E = mc^2$
This equation, E=mc², was derived by Albert Einstein as a part of his theory of special relativity in 1905. It states that mass and energy are interchangeable, altering forever the way we understand the universe. It also led to the development of nuclear energy and nuclear weapons.
HEISENBERG'S UNCERTAINTY PRINCIPLE
(QUANTUM MECHANICS)
$\Delta x \Delta p \geq \frac{\hbar}{2}$
Formulated by Werner Heisenberg in 1927, the uncertainty principle is one of the core tenets of quantum mechanics. It states that the more precisely the position of a particle is determined, the less precisely its momentum can be known, and vice versa. It underpins the inherently probabilistic nature of quantum mechanical phenomena.
DIRAC EQUATION
(QUANTUM FIELD THEORY)
$(i\hbar\gamma^\mu\partial_\mu - mc)\psi = 0$
Proposed by Paul Dirac in 1928, this equation describes fermions—particles with half-integer spin—and led to the prediction of antimatter. It's critical in quantum field theory and has shaped our understanding of the fundamental nature of particles and the universe.
EULER'S IDENTITY
(COMPLEX ANALYSIS)
$e^{i\pi} + 1 = 0$
Named after the Swiss mathematician Leonhard Euler, this identity is a special case of Euler's formula from complex analysis, and it beautifully combines five of the most important numbers in mathematics: 0, 1, π, e, and i. It's considered by many to be the most beautiful equation in mathematics due to its elegant linking of these fundamental numbers.
MAXWELL'S EQUATIONS
(ELECTRODYNAMICS)
$\nabla \cdot \mathbf{D} = \rho$
$\nabla \cdot \mathbf{B} = 0$
$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$
$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$
Formulated by James Clerk Maxwell and Oliver Heaviside in 1862, these four equations describe how electric and magnetic fields interact. They underpin all of classical electrodynamics, optics, and electric circuits and paved the way for the advent of technologies such as radio, television, and radar.
EINSTEIN'S FIELD EQUATIONS
(GENERAL RELATIVITY)
$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R + g_{\mu\nu}\Lambda = \frac{8\pi G}{c^4}T_{\mu\nu}$
Published by Albert Einstein in 1915, these equations describe how matter and energy in the Universe distort spacetime to create the phenomenon we experience as gravity. They are fundamental to cosmology and astrophysics, predicting phenomena like gravitational waves and black holes.
SCHRODINGER EQUATION
(QUANTUM MECHANICS)
$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$
Proposed by Erwin Schrödinger in 1926, this equation describes how the quantum state of a quantum system changes with time. It forms the basis of quantum mechanics and has been crucial in the development of many modern technologies, from semiconductors to MRI scanners.


The first time you read about quantum mechanics:
The 1000th time you read about quantum mechanics:


Twitter Books
@TwitterBooks
Last book that made you cry
4:52 PM · 1/27/20 · Sprinklr
23 Retweets 144 Likes
[redacted]
Replying to @TwitterBooks
University Physics with Modern Physics 14th Edition by Hugh D. Young, Roger A. Freedman
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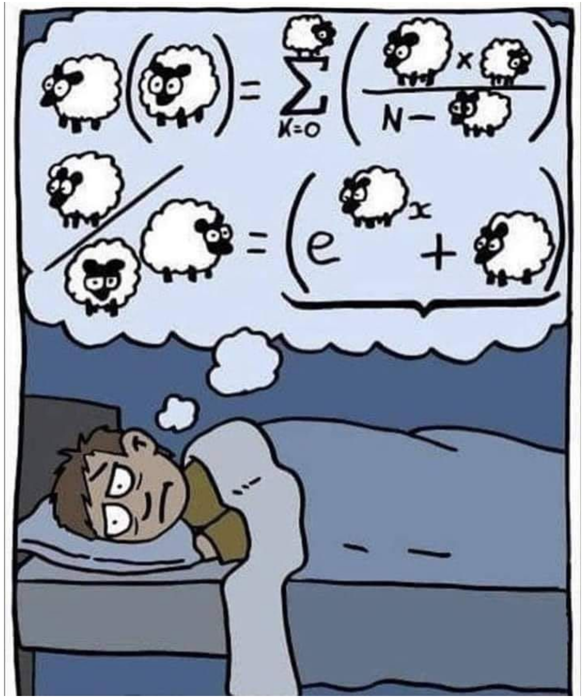
3
Roger Freedman @RogerFreed... · 5h
No doubt tears of joy.



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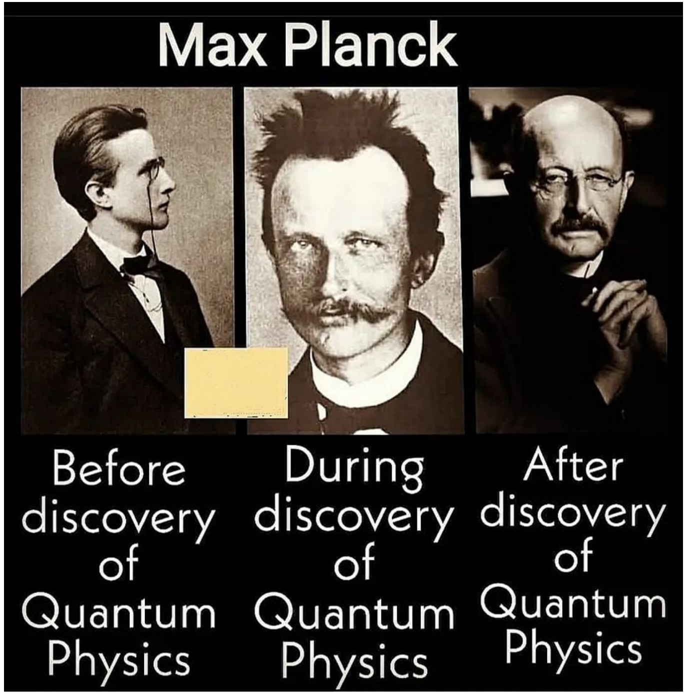
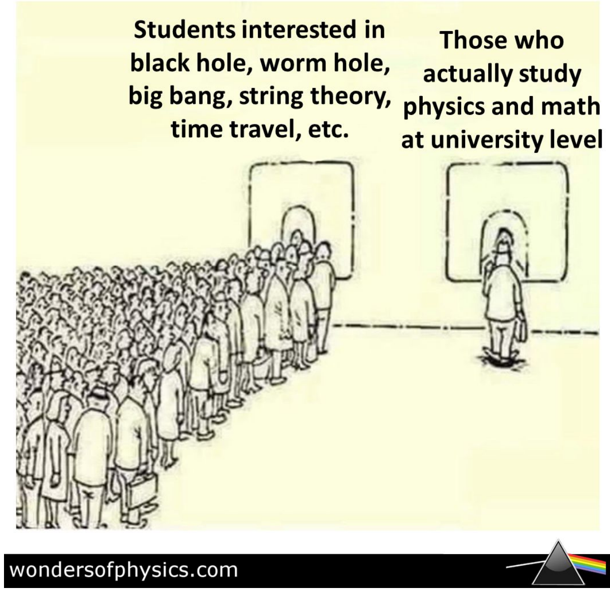
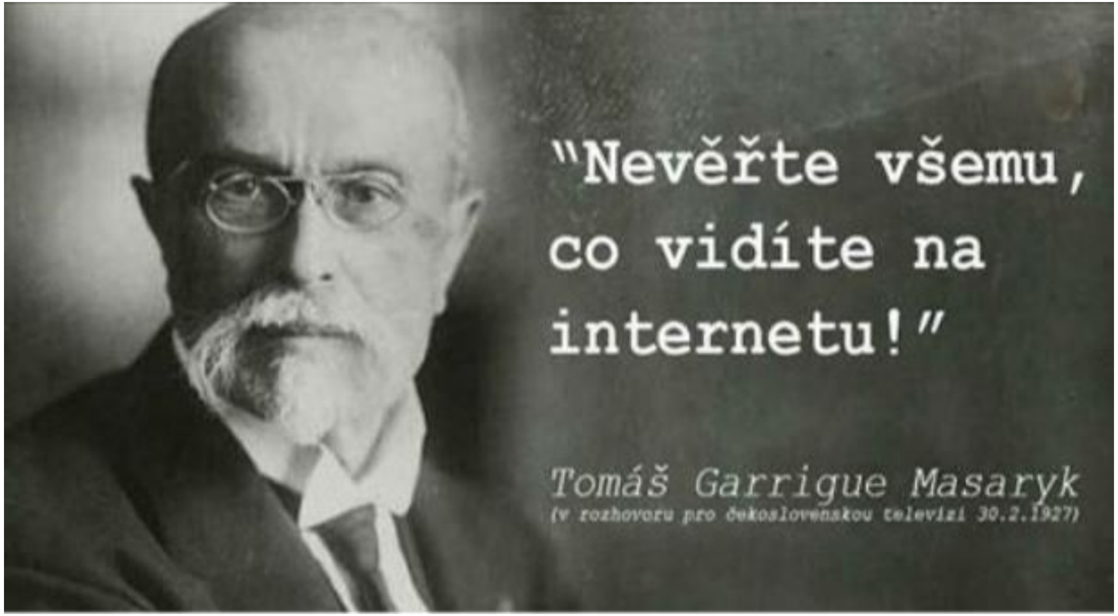


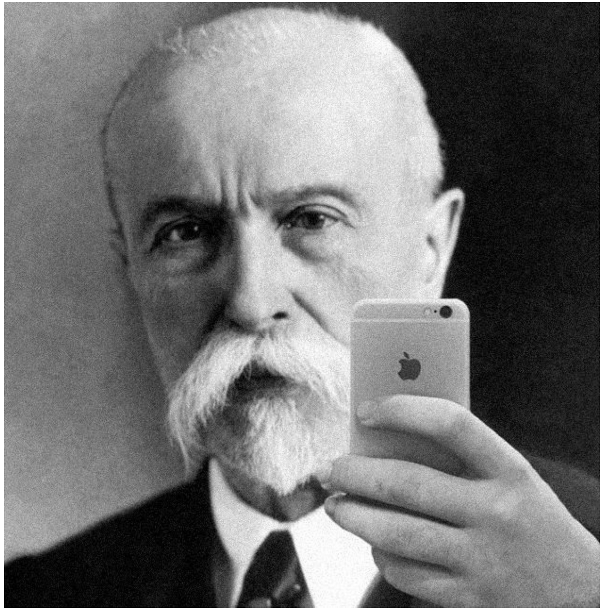
Max Planck
Before discovery of Quantum Physics
During discovery of Quantum Physics
After discovery of Quantum Physics



Students interested in black hole, worm hole, big bang, string theory, time travel, etc.
Those who actually study physics and math at university level
wondersofphysics.com

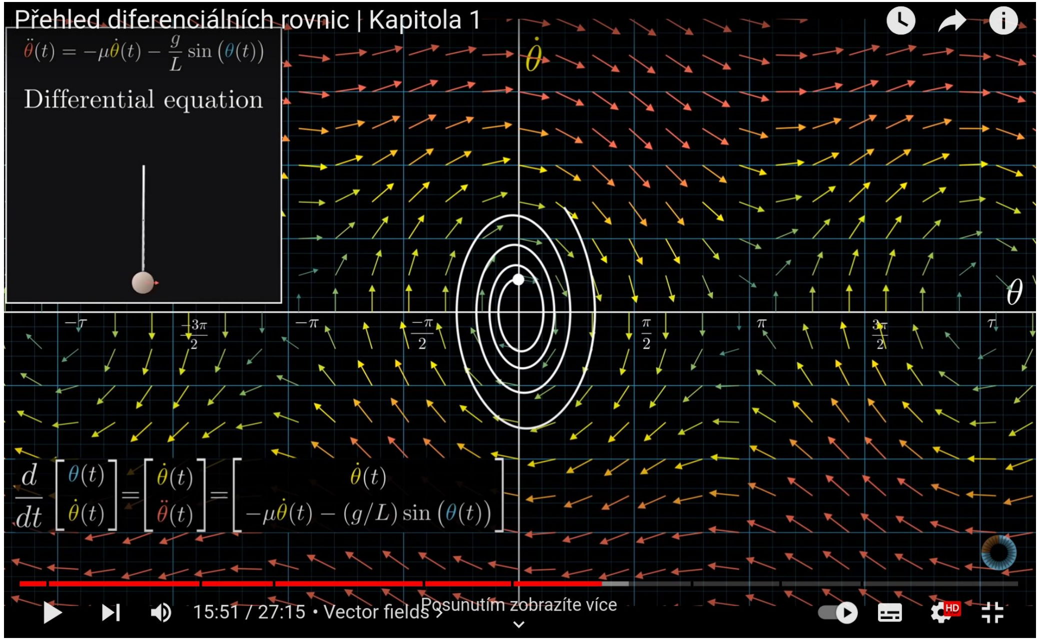
A gentle reminder…





Diferenciální rovnice @ 3B1B

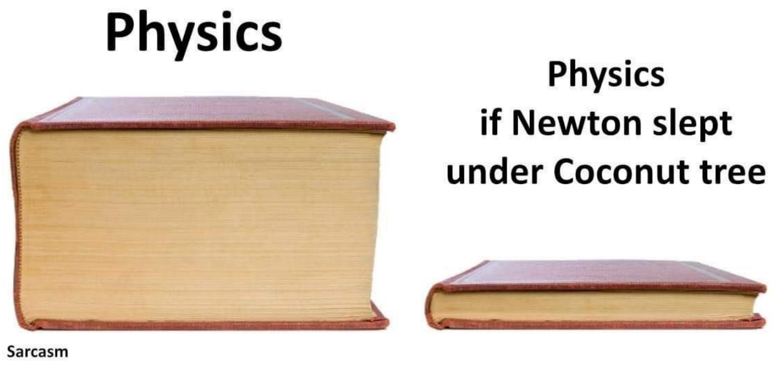
https://www.youtube.com/watch?v=p_di4Zn4wz4&t=802s&ab_channel=3Blue1Brown

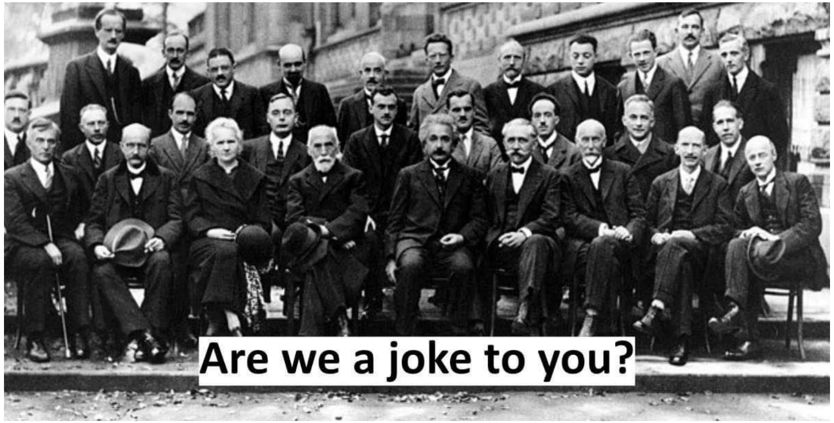


Backup

1927 :: https://en.wikipedia.org/wiki/Solvay_Conference

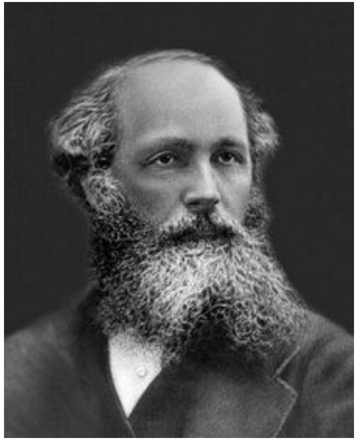
Midjourney





Maxwellovy rovnice

- Rovnice popisující elektromagnetická pole.
- Popisují mj. i elektromagnetické vlny.
- Jsou invariantní vůči relativistické Lorentzově transformaci!



James Clerk Maxwell

$$\operatorname{div} \vec{B} = 0 \qquad \operatorname{div} \vec{E} = \frac{\rho}{\varepsilon_0}$$

$$\operatorname{rot} \vec{B} = \mu_0 \left(\varepsilon_0 \frac{\partial \vec{E}}{\partial t} + \vec{j} \right) \qquad \operatorname{rot} \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

Maxwellovy rovnice

$$A^\mu \equiv \left(\frac{1}{c}\phi, \vec{A} \right) \qquad \vec{B} = \mathrm{rot}\,\vec{A}$$

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \qquad \vec{E} = -\mathrm{grad}\,\phi - \frac{\partial \vec{A}}{\partial t}$$

$$\partial_\alpha F^{\alpha\beta} = \mu_0 J^\beta$$

Vakuum: $\partial_\alpha F^{\alpha\beta} = 0$

$$F^{\mu\nu} = \begin{pmatrix} 0 & -\frac{E_x}{c} & -\frac{E_y}{c} & -\frac{E_z}{c} \\ \frac{E_x}{c} & 0 & -B_z & B_y \\ \frac{E_y}{c} & B_z & 0 & -B_x \\ \frac{E_z}{c} & -B_y & B_x & 0 \end{pmatrix}$$

Pauliho rovnice

- Rozšíření nerelativistické Schrödingerovy rovnice pro částici se spinem ½
- Vlnová funkce má 2 komponenty popisující 2 možné stavy (projekce) spinu.

Wolfgang Pauli

Pauli:

$$H = \frac{1}{2m}\left[\left(\vec{p} - q\vec{A}\right)^2 - \hbar q\, \vec{\sigma}\cdot\vec{B}\right] + q\phi$$

$$= \frac{1}{2m}\left[\vec{\sigma}\cdot\left(\vec{p} - q\vec{A}\right)\right]^2 + q\phi$$

Klein – Gordonova rovnice – relativistická

- Relativistická rovnice popisující částici se spinem 0.
  - Inspirací je vztah $E^2 = m^2c^4 + p^2c^4$.
  - Spin je vnitřní moment hybnosti částice
  - Ale elektron má spin ½ …
  - A rovnice má některé nehezké vlastnosti…

Oskar Benjamin Klein

$$\hat{\vec{p}} = -i\hbar\nabla \qquad \hat{\vec{p}}^2 = -\hbar^2\Delta$$

$$E^2 = m^2c^4 + \vec{p}^2c^2 \qquad E \sim i\hbar\frac{\partial}{\partial t} \qquad i^2 = -1$$

$$\Rightarrow \left[-\hbar^2c^2\Delta + m^2c^4\right]\psi = -\hbar^2\frac{\partial^2}{\partial t^2}\psi$$

Klein – Gordonova rovnice – relativistická

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Oskar Benjamin Klein

Klein - Gordon: $$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \Delta\psi + \frac{m^2c^2}{\hbar^2}\psi = 0$$

$$\left[\frac{1}{c^2}\partial_t^2 - \Delta + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0$$

$\hbar = c = 1$: $$(\Box + m^2)\psi = 0$$

Diracova rovnice – relativistická rovnice QM

- Ukazuje se, že popisuje částici se spinem ½
  - tj. např. elektron
  - vlnová funkce zde má 4 komponenty
  - předpovídá existenci antičástic
- Demokratická v prostoru a čase, první derivace podle obou.

$$\left[\vec{\alpha}\cdot\hat{\vec{p}}c + \beta mc^2\right]\psi(\vec{x},t) = i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t}$$

$$\left[-i\hbar c\,\vec{\alpha}\cdot\nabla + \beta mc\right]\psi = i\hbar\frac{\partial}{\partial t}\psi$$

$$\nabla \equiv \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$$

$\vec{\alpha}, \beta$ ... matice

$$\psi \equiv \psi(\vec{x},t) = \begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}$$

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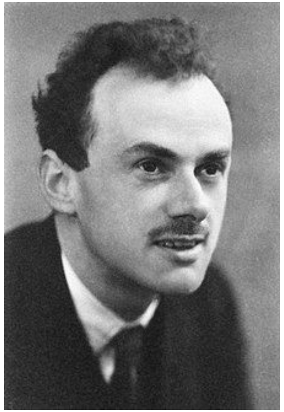


Paul A. M. Dirac

Dirac $\left(i\hbar\,\gamma^{\mu}\partial_{\mu} - mc\right)\psi = 0$

$\hbar = c = 1$ $\left(i\not{\partial} - m\right)\psi = 0$

$H = \vec{\alpha}\cdot\vec{p}c + \beta mc^2 \quad : \quad H^2 = p^2c^2 + m^2c^4$

$\sqrt{a^2+b^2} = a + b$:-)

$\vec{\gamma} = \beta\vec{\alpha} \qquad \gamma^0 = \beta$

$\gamma^{\mu} = (\gamma^0, \vec{\gamma}) \qquad a^{\mu}\gamma_{\mu} \equiv \not{a}$

$\psi = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} \qquad \psi : \mathbb{R}^{3,1} \longmapsto \mathbb{C}^4$

Princip stacionární akce

- Akce je integrál z Lagrangiánu
- Lagrangián je rozdílem kinetické a potenciální energie
  - ale je to funkce funkcí popisujících trajektorii:)
- Princip vede na Euler-Lagrangeovy rovnice, které vedou na Newtonovy.
  - vyhýbají se konceptu síly, pracují s potenciálem!

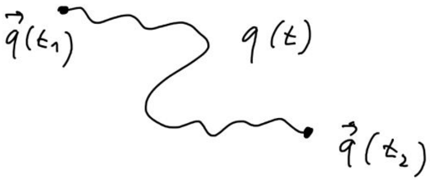
Joseph-Louis Lagrange

$$\delta S = 0 \qquad S = \int_{t_1}^{t_2} L(q, \dot{q}, t)\, dt$$

$$S = \int \mathcal{L}(\phi, \partial_\sigma \phi, t)\, d^4x$$

$$L = T - V$$

$$\mathcal{L} = \mathcal{T} - \mathcal{V}$$



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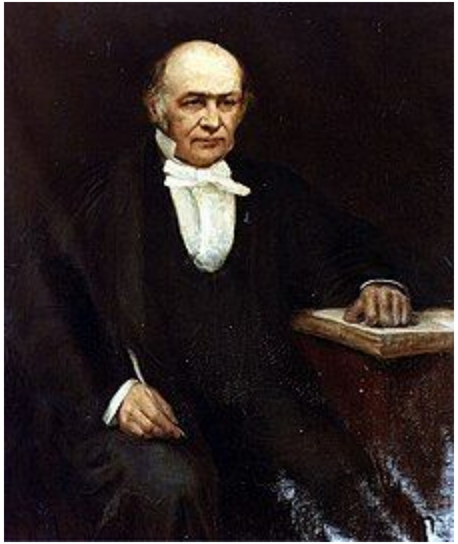
Joseph-Louis Lagrange

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0$$

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi} - \frac{\partial \mathcal{L}}{\partial \phi} = 0$$

Hamiltonovy rovnice

- Zavádějí hybnost jako nezávislou proměnnou
- Hamiltonián je funkcionál celkové energie
- Cesta k zobecnění do kvantové mechaniky! :-)



Sir William Rowan Hamilton

$$p \equiv \frac{\partial L}{\partial \dot{q}}$$

$$H = p\dot{q} - L \equiv H(p, q, t)$$

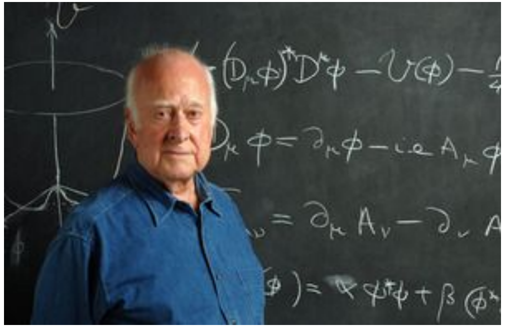
$$\frac{\partial H}{\partial q} = -\dot{p} \qquad \frac{\partial H}{\partial p} = \dot{q}$$

$$H = T + V = T(p) + V(q)$$

$$H = \frac{p^2}{2m} + V(q) \qquad E_k = T = \frac{1}{2} m v^2 = \frac{p^2}{2m}$$

Standardní Model

- Lagrangián Standardního Modelu
- Kinetické a interakční členy
- Higgsův potenciál
- Seldon Glashow, Steven Weinberg, David Politzer, David Gross, Frank Wilczek, Abdus Salam



$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} \cdot F_{\mu\nu}$$
$$+ i \bar{\psi} \not{D} \psi + h.c.$$
$$+ \bar{\psi}_i y_{ij} \psi \phi + h.c.$$
$$+ (D_\mu \phi)^\dagger (D^\mu \phi)$$
$$+ \mu^2 \phi^\dagger \phi - \lambda (\phi^\dagger \phi)^2$$