Posebna teorija relativnosti

Einsteinova postulata relativnosti:

1. Fizikalni zakoni imajo enako obliko v vseh inerc. sistemih.
2. Hitrost svetlobe v vakuumu je enaka v vseh inerc. sistemih.

$\beta_v = \frac{v}{c} \qquad \gamma_v = (1-\beta_v^2)^{-\frac{1}{2}}$

$$\Lambda^\mu_\nu = \begin{bmatrix} \gamma_v & -\beta_v\gamma_v & 0 & 0 \\ -\beta_v\gamma_v & \gamma_v & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$x^\mu = (ct, x, y, z) = (x^0, x^1, x^2, x^3)$ (svetovni četverec)
$x^\mu = \Lambda^\mu_\nu \, x^\nu \qquad x^\nu = \Lambda^\nu_\mu \, x^\mu$ (Lorentzova transformacija)
$u_x' = \frac{u_x - v}{1-\frac{u_x v}{c^2}} \qquad u_y' = \frac{u_y}{\gamma_v\left(1-\frac{u_x v}{c^2}\right)}$
$a_x' = a_x\left(\gamma_v^3\left(1-\frac{u_x v}{c^2}\right)^3\right)^{-1}$
$a_y' = \left(\gamma_v^2\left(1-\frac{u_x v}{c^2}\right)^3\right)^{-1}\left[\left(1-\frac{u_x v}{c^2}\right)a_y + \frac{v}{c^2}u_y a_x\right]$

$l' = l/\gamma$ (skrčenje dolžin)
$t' = \gamma\tau$ (podaljšanje časa)

$a_\mu = (a^0, -a^1, -a^2, -a^3)$
$a^\mu \cdot b_\mu = a^0 b^0 - a^1 b^1 - a^2 b^2 - a^3 b^3$
$x^\mu x_\mu = (x^\mu)^2$ je invarianten proti Lorentozvi transformaciji

1. $(\Delta x^\mu)^2 > 0$ dogodek časovnega tipa - $\exists S : t_1 \neq t_2, \vec{r}_1 = \vec{r}_2$,
2. $(\Delta x^\mu)^2 = 0$ dogodek svetlobnega tipa,
3. $(\Delta x^\mu)^2 < 0$ dogodek krajevnega tipa - $\exists S : t_1 = t_2, \vec{r}_1 \neq \vec{r}_2$.

Zakoni gibanja

$u^\mu = \frac{dx^\mu}{d\tau} = \gamma_u \frac{dx^\mu}{dt} = (\gamma_u c, \gamma_u \vec{u})$ (četverec hitrosti)
$u^\mu = \Lambda^\mu_\nu \, u^\nu \qquad u^\nu = \Lambda^\nu_\mu \, u^\mu$
$u^\mu \cdot u_\mu = c^2$ (invarianta)

$p^\mu = m u^\mu = (\gamma_u mc, m\gamma_u u) = (E/c, \vec{p})$ (četverec GK)
$p^\mu = \Lambda^\mu_\nu \, p^\nu \qquad p^\nu = \Lambda^\nu_\mu \, p^\mu$
$T = E - E_0 = \gamma mc^2 - mc^2 = (\gamma - 1)mc^2$
$E^2 = c^2 p^2 + m^2 c^4$

$\vec{F} = \frac{d\vec{p}}{dt} = m\gamma\vec{a} + m\gamma^3 \frac{\vec{a}\cdot\vec{v}}{c^2}\vec{v}$
$F^\mu = \frac{dp^\mu}{d\tau} = (\gamma\frac{\vec{F}\cdot\vec{u}}{c}, \gamma\vec{F})$ (sila Minkowskega)
$a^\mu = \frac{du^\mu}{d\tau} = (\gamma^4 \frac{\vec{a}\cdot\vec{v}}{c}, \gamma^2\vec{a} + \gamma^4 \frac{\vec{a}\cdot\vec{v}}{c^2}\vec{v})$ (četverec pospeška)
$F^\mu = m a^\mu$

Sistemi delcev

$\beta^* = \frac{c\sum p_i}{\sum E_i}$ (težiščni sistem)
$p_0^\mu \cdot p_{\mu 0} = p^\mu \cdot p_\mu = p_0^{\mu *} \cdot p_{\mu 0}^* = p^{\mu *} \cdot p_\mu^*$

Popolnoma neprožni trk: $M = \sqrt{2(\gamma+1)}m$

Razpoložljiva energija pri fiksni tarči:
$E_r = Mc^2 - 2mc^2 = 2mc^2\left(\sqrt{\frac{\gamma+1}{2}} - 1\right)$

Elektromagnetno polje

$\mathcal{E}_x' = \mathcal{E}_x$
$\mathcal{E}_y' = \gamma(\mathcal{E}_y - \beta c B_z)$
$\mathcal{E}_z' = \gamma(\mathcal{E}_z + \beta c B_y)$

$B_x' = B_x$
$B_y' = \gamma(B_y + \beta\mathcal{E}_z/c)$
$B_z' = \gamma(B_z - \beta\mathcal{E}_y/c)$

$\vec{E}\cdot\vec{B} = konst.$
$\vec{E}\cdot\vec{E} - c^2\vec{B}\cdot\vec{B} = konst.$

$j^\mu = (c\rho_e, \vec{j}_e)$

$$F^{\mu\nu} = \begin{bmatrix} 0 & -\mathcal{E}_x/c & -\mathcal{E}_y/c & -\mathcal{E}_z/c \\ \mathcal{E}_x/c & 0 & -B_z & B_y \\ \mathcal{E}_y/c & B_z & 0 & -B_x \\ \mathcal{E}_z/c & -B_y & B_x & 0 \end{bmatrix}$$

$\frac{dp^\mu}{d\tau} = eF^{\mu\nu}u_\nu$

Dopplerjev pojav:

1. $\nu_o = \nu_s \frac{\sqrt{1-\beta_v^2}}{1-\beta_v\cos\vartheta}$
2. $\vartheta = 0 : \nu_o = \nu_s\sqrt{\frac{1+\beta_v}{1-\beta_v}}$
3. $\vartheta = \frac{\pi}{2} : \nu_o = \nu_s\sqrt{1-\beta_v^2}$

Kvantna fizika

Kvantni pojavi s fotoni

Sevanje črnega telesa:
$\frac{dw}{d\nu} = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{h\nu/kT}-1}$
$\frac{dw}{d\lambda} = \frac{8\pi hc}{\lambda^5}\frac{1}{e^{hc/\lambda kT}-1}$
$j = \frac{1}{4}cw = \sigma T^4$
$\lambda_{\max} T = k_W$

Fotoelektrični pojav: $E_{\max} = h\nu - \Phi$

Rentgensko sevanje: $e_0 U = h\nu_{\max}$

Comptonov pojav: $\lambda_c = \frac{h}{m_e c}$
$\lambda' - \lambda = \lambda_c(1-\cos\vartheta)$

Valovanje delcev

$p = \frac{h}{\lambda} = \hbar k$
$E = h\nu = \hbar\omega$
Imamo disperzijo, grupna hitrost valovanja se ujema s hitrostjo delca (v klasičnem in relativističnem).

Bragg: $2d\cos\vartheta = n\lambda$ (sipalni kot, sin, če je vpadni)

$\rho(x,t) = \frac{d^2N}{N dt dx} = \Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2$
$P(\text{delec na } [a,b]) = \frac{\Delta N}{N} = \int_a^b \rho(x)\,dx$
$\int_{-\infty}^{\infty}\rho(x)\,dx = 1$

Valovni paket:
$\Psi(x,t) =$
$A\lim_{N\to\infty}\sum_{n=-N}^{N}\exp\{-i\left[\left(\omega + \frac{n}{N}\Delta\omega\right)t - \left(k + \frac{n}{N}\Delta k\right)x\right]\} =$
$= Ae^{-i(\omega t - kx)}N\frac{2i\sin(\Delta\omega t - \Delta kx)}{-i(\Delta\omega t - \Delta kx)}$
$\rho(x,t) = 4|A|^2 N^2 \frac{\sin^2(\Delta\omega t - \Delta kx)}{(\Delta\omega t - \Delta kx)^2}$

Gaussov valovni paket:
$\psi(x) = \int_{-\infty}^{\infty} A_0\exp\left(\frac{-(k-k_0)^2}{4\sigma_k^2}\right)e^{ikx}\,dx =$
$= \frac{\sqrt{2}}{2}\frac{1}{\sigma_x}A_0\exp\left(\frac{-x^2}{4\sigma_x^2}\right)e^{ik_0x}, \qquad \sigma_x = \frac{1}{2\sigma_k}$
$\rho(x) \propto \exp\left(\frac{-x^2}{4\sigma_x^2}\right)$

Heisenbergovo načelo nedoločenosti:
$\sigma_x\sigma_p \geq \frac{\hbar}{2} = \frac{h}{4\pi}$
$\sigma_E\sigma_t \geq \frac{\hbar}{2} = \frac{h}{4\pi}$
$\sigma^2 = \langle x^2\rangle - \langle x\rangle^2$

Nerelativistična kvantna mehanika v 1D

$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$
$\hat{H}\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$ (Nestacionarna Schrödingerjeva enačba)
$\hat{H}\psi(x) = E\psi(x)$ (Stacionarna Schrödingerjeva enačba)
$\Psi(x,t) = \psi(x)\exp\left(-\frac{iE}{\hbar}t\right)$

$j(x,t) = \frac{\hbar}{2mi}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)$
$\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x}j(x,t) = 0$

Ψ je vedno zvezna, Ψ' je vedno zvezna, razen v točkah kjer $V\to\infty$ ali $V\sim\delta(x)$.
$\langle\psi_m,\psi_n\rangle = \int_{-\infty}^{\infty}\psi_n^*\psi_m\,dx = \delta_{mn}$
ψ_n, ψ_m rešitvi SSE $\implies c_n\psi_n + c_m\psi_m$ rešitev SSE.

Vsako rešitev SSE lahko razvijemo po lastnih $\psi = \sum c_n\psi_n$.
$\sum|c_n|^2 = 1$
$c_m = \int_{-\infty}^{\infty}\psi_m^*\psi\,dx$
$\Psi = \sum c_n\psi_n\exp\left(-\frac{iE_n}{\hbar}t\right)$

Neskončna potencialna jama:
$V = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{sicer} \end{cases}$
$E_1 = \frac{\pi^2\hbar^2}{2ma^2} \qquad E_n = n^2 E_1$
$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(n\frac{\pi}{a}x\right)$

Linearni harmonični oscilator:
$V = \frac{1}{2}kx^2 = \frac{1}{2}m\omega_0^2x^2$
$E_n = \hbar\omega_0(n + \frac{1}{2})$
$\psi_n(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}}\left(\frac{1}{2^n n!}\right)^{\frac{1}{2}}H_n\left[\left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}}x\right]e^{-m\omega_0x^2/2\hbar}$
H_n so Hermitovi polinomi.
$\hat{x}\psi_n = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n+1}\psi_{n+1} + \sqrt{n}\psi_{n-1})$
$\hat{x}^2\psi_n =$
$\frac{\hbar}{2m\omega}(\sqrt{(n+1)(n+2)}\psi_{n+2} + (2n+1)\psi_n + \sqrt{n(n-1)}\psi_{n-2})$

Curek delcev:
$\psi = Ae^{ikx} \implies p_x = \hbar k, \quad E = \frac{p_x^2}{2m} = \frac{\hbar^2k^2}{2m}$
$j = |A|^2 v$

V splošnem: $\psi = Ae^{ikx} + Be^{-ikx}$
$j = \frac{\hbar k}{m}(A^*A - B^*B)$

Potencialna stopnica:
$$V = \begin{cases} 0 & x < 0 \\ V_0 = \text{konst.} \neq 0 & x > 0 \end{cases}$$
$$\psi = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{ik_2x} + (De^{-ik_2x}) & x > 0 \end{cases}$$
$k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$
$B = \frac{k_1-k_2}{k_1+k_2}A \qquad C = \frac{2k_1}{k_1+k_2}A$
$R = \frac{j_{\text{odbita}}}{j_{\text{vpadna}}} = |\frac{B}{A}|^2 = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2$
$T = \frac{j_{\text{prep.}}}{j_{\text{vpadna}}} = \frac{|C|^2k_2}{|A|^2k_1} = \frac{4k_1k_2}{(k_1+k_2)^2}$
$R + T = 1$

$$F_{ij} = \frac{1}{2}\begin{bmatrix} 1 + \frac{k_j}{k_i} & 1 - \frac{k_j}{k_i} \\ 1 - \frac{k_j}{k_i} & 1 + \frac{k_j}{k_i} \end{bmatrix}$$
$$\begin{bmatrix} A \\ B \end{bmatrix} = F_{12}\begin{bmatrix} C \\ D \end{bmatrix}$$

Potencialna plast:
$$V = \begin{cases} 0 & x < 0 \\ V_0 = \text{konst.} \neq 0 & 0 < x < a \\ 0 & x > a \end{cases}$$
$$\psi = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x < 0 \\ Ce^{ik_2x} + De^{-ik_2x} & 0 < x < a \\ Fe^{ik_1x} + (Ge^{-ik_1x}) & x > a \end{cases}$$
$k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$
$C = \frac{1}{2}\left(1 + \frac{k_1}{k_2}\right)e^{i(k_1-k_2)a}A$
$D = \frac{1}{2}\left(1 - \frac{k_1}{k_2}\right)e^{i(k_1+k_2)a}A$
$F = \frac{2k_1k_2e^{-ik_1a}}{2k_1k_2\cos(k_2a) - i(k_1^2+k_2^2)\sin(k_2a)}A$
$B = \frac{-i(k_1^2+k_2^2)\sin(k_2a)}{2k_1k_2\cos(k_2a) - i(k_1^2+k_2^2)\sin(k_2a)}A$
$T = \frac{j_{\text{prep.}}}{j_{\text{vpadna}}} = |\frac{F}{A}|^2 = \left[1 + \frac{1}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)^2\sin^2(k_2a)\right]^{-1}$
$R = \frac{j_{\text{odbita}}}{j_{\text{vpadna}}} = |\frac{C}{A}|^2 = 1 - T$

$$\Phi = \begin{bmatrix} e^{ik_2a} & 0 \\ 0 & e^{-ik_2a} \end{bmatrix}$$
Z Φ popravimo fazo, predstavljamo si, da je novo koordinatno izhodišče pri $x = a$, kjer imamo še en prehod čez potencialno stopnico.
$$\begin{bmatrix} F \\ G \end{bmatrix} = F_{32}\Phi F_{21}\begin{bmatrix} A \\ B \end{bmatrix}$$

Operatorji in pričakovane vrednosti

$\langle\hat{A}\rangle = \int_{-\infty}^{\infty}\Psi^*\hat{A}\Psi\,dV$
$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$
$\hat{T}_x = \frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$\hat{E} = \hat{H} = \hat{T} + \hat{V} = i\hbar\frac{\partial}{\partial t}$

Operatorji dinamičnih spremenljivk morajo biti sebi-adjungirani.
Lastne funkcije takih operatorjev so ortogonalne.
$\int(\hat{A}\psi_n)^*\psi_n\,dV = \int\psi_n^*\hat{A}\psi_n\,dV$

Ob razvoju po lastnih funkcijah: $\langle E\rangle = \sum|c_n|^2E_n$
$\implies |c_n|^2$ verjetnost za meritev energije E_n v danem stanju.

$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ (komutator)
$\sigma_A\sigma_B \geq \frac{1}{2}|\langle[\hat{A},\hat{B}]\rangle|$
$\frac{d\langle\hat{A}\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle$

Nerelativistična kvantna mehanika v 3D

$\hat{\vec{p}} = -i\hbar\nabla$
$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$
$\Psi(\vec{r},t), \psi(\vec{r})$, SSE in NSE enaki kot v 1D

Neskončna potencialna jama:
$$V = \begin{cases} 0 & 0 \leq x \leq a, 0 \leq y \leq b, 0 \leq z \leq c \\ \infty & \text{sicer} \end{cases}$$
$E_{n_xn_yn_z} = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$
$\psi_{n_xn_yn_z}(\vec{r}) = \sqrt{\frac{8}{abc}}\sin\left(n_x\frac{\pi}{a}x\right)\sin\left(n_y\frac{\pi}{b}y\right)\sin\left(n_z\frac{\pi}{c}z\right)$

Linearni harmonični oscilator:
$V = \frac{1}{2}kr^2 = \frac{1}{2}m\omega_0^2(x^2+y^2+z^2)$
$E_{n_xn_yn_z} = \hbar\omega_0(n_x + n_y + n_z + \frac{3}{2})$
$\psi_n^{3d}(x) = \psi_{n_x}^{1d}(x)\psi_{n_y}^{1d}(y)\psi_{n_z}^{1d}(z)$
Degeneracija izgine, ko zlomimo simetrijo (k ni enak za vse).

Vrtilna količina

$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = -i\hbar\left(-\sin\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\cos\varphi\frac{\partial}{\partial\varphi}\right)$
$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = -i\hbar\left(\cos\varphi\frac{\partial}{\partial\vartheta} - \cot\vartheta\sin\varphi\frac{\partial}{\partial\varphi}\right)$
$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\varphi}$
$\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2\left(\frac{\partial^2}{\partial\vartheta^2} + \cot\vartheta\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right)$

$[\hat{L}_x,\hat{L}_y] = -i\hbar\hat{L}_z, \quad [\hat{L}_y,\hat{L}_z] = -i\hbar\hat{L}_x, \quad [\hat{L}_z,\hat{L}_x] = -i\hbar\hat{L}_y$
$[\hat{\vec{L}}^2,\hat{L}_x] = 0, \quad [\hat{\vec{L}}^2,\hat{L}_y] = 0, \quad [\hat{\vec{L}}^2,\hat{L}_z] = 0$
$[\hat{\varphi},\hat{L}_z] = i\hbar \quad \implies \quad \sigma_\varphi\sigma_{L_z} \geq \frac{\hbar}{2}$

$\hat{L}_z\Phi(\varphi) = L_z\Phi(\varphi)$
$\Phi_{m_l}(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im_l\varphi}$
$L_z = m_l\hbar, \quad m_l = 0, \pm1, \pm2\ldots$

$\hat{\vec{L}}^2Y(\vartheta,\varphi) = \vec{L}^2Y(\vartheta,\varphi)$
$Y_{lm_l}(\vartheta,\varphi) = \Theta_{lm_l}(\vartheta)\Phi_{m_l}(\varphi) = A_{lm_l}P_l^{m_l}(\cos\vartheta)e^{im_l\varphi}$
$\int Y_{lm_l}^*Y_{l'm_l'}\,d\Omega = \delta_{ll'}\delta_{m_lm_l'}$
$\vec{L}^2 = l(l+1)\hbar^2, \quad |m_l| \leq l$
$P_l^{m_l}$ so pridruženi Legendrovi polinomi.

$\langle l'm_l'|\,\hat{L}_z\,|lm_l\rangle = m\hbar\delta_{ll'}\delta_{m_lm_l'}$

$\langle l'm_l'|\,\hat{\vec{L}}^2\,|lm_l\rangle = \hbar^2l(l+1)\delta_{ll'}\delta_{m_lm_l'}$
$\langle l'm_l'|\,\hat{L}_x\,|lm_l\rangle = \frac{\hbar}{2}\sqrt{l(l+1) - m(m\pm1)}\delta_{ll'}\delta_{m_l(m_l'\pm1)}$
$\langle l'm_l'|\,\hat{L}_x\,|lm_l\rangle = \mp\frac{i\hbar}{2}\sqrt{l(l+1) - m(m\pm1)}\delta_{ll'}\delta_{(m_l\pm1)m_l'}$

Rotator
$E_{\text{rot}} = \frac{\vec{L}^2}{2J} = \frac{\hbar^2}{2J}l(l+1)$
Degeneracija je $2l+1$ kratna.
Lastne funkcije so Y_{lm_l}

Enoelektronski atom

$r_B = \frac{4\pi\varepsilon_0\hbar^2}{m_ee_0^2}$
$r_n = n^2\frac{r_B}{Z}$
$E_0 = \frac{m_ek^2e_0^4}{2\hbar^2}, \qquad k = \frac{1}{4\pi\varepsilon_0}$

$V(r) = \frac{-Ze_0^2}{4\pi\varepsilon_0r}$
$\hat{H} = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2}\right) - \frac{\alpha\hbar c}{r}$
$\mu = \frac{m_eM}{m_e+M}$
$a = \frac{m_e}{\mu}\frac{r_B}{Z}$
$E_n = -\frac{\mu}{m_e}\frac{Z^2}{n^2}E_0$
$\Psi_{nlm_l}(r,\vartheta,\varphi,t) = R_{nl}(r)Y_{lm_l}(\vartheta,\varphi)e^{-iE_nt/\hbar}$
$R_{nl}(r) = A_{nl}r^lL_{nl}(\frac{r}{nr_B})e^{-\frac{r}{nr_B}}$
$R_{nl}(0)$ ima l-kratno ničlo.
$\int\psi_{nlm_l}^*\psi_{n'l'm_l'}\,d\Omega = \delta_{nn'}\delta_{ll'}\delta_{m_lm_l'}$
L_{nl} so posplošeni Laguerrovi polinomi.

$n = 1, 2\ldots$
$0 \leq l \leq n-1, \quad l \in \mathbb{Z}$
$|m_l| \leq l, \quad m_l \in \mathbb{Z}$
Degeneracija je n^2 kratna.

$\langle r\rangle = an^2\left(1 + \frac{1}{2}\left[1 - \frac{l(l+1)}{n^2}\right]\right)$
$\langle\frac{1}{r}\rangle = \frac{1}{an^2}$
$\langle\frac{1}{r^2}\rangle = \frac{1}{a^2n^3(2l+1)}$
$\langle\frac{1}{r^3}\rangle = \frac{1}{a^3n^3(2l+1)(l+1)}$
$\langle V\rangle = -\frac{Ze_0^2}{4\pi\varepsilon_0}\langle\frac{1}{r}\rangle = -Z^2\left(\frac{e_0^2}{4\pi\varepsilon_0}\right)^2\frac{\mu}{\hbar^2n^2}$
$\langle E\rangle = -\frac{Z^2}{2}\left(\frac{e_0^2}{4\pi\varepsilon_0}\right)^2\frac{\mu}{\hbar^2n^2}$
$\langle T\rangle = \langle E\rangle - \langle V\rangle = -\frac{1}{2}\langle V\rangle$

Atom v magnetnem polju

$\hat{\vec{\mu}}_l = -\frac{e_0}{2m_e}\hat{\vec{L}} = -g_l\mu_B\frac{\hat{\vec{L}}}{\hbar} \qquad (g_l = 1)$
Lastne funkcije $\hat{\vec{\mu}}_l$ so lastne funkcije $\hat{\vec{L}}$.
$\mu_l = g_l\sqrt{l(l+1)}\mu_B$
Lastne funkcije $\hat{\mu}_{lz}$ so lastne funkcije $\hat{L}_z$.
$\mu_{lz} = g_lm_l\mu_B$
$\vec{\omega}_L = \frac{|e|\vec{B}}{2m_e}$ (Larmanova frekvenca)
$F_z = -\frac{\partial E_{\text{mag}}}{\partial z} = -\mu_z\frac{\partial B}{\partial z}$

$\hat{H}_{\mathrm{mag}} = -\hat{\vec{\mu}}_l \cdot \vec{B} = -\hat{\mu}_{lz} B_z$

Spin

$[\hat{S}_x, \hat{S}_y] = -i\hbar \hat{S}_z, \quad [\hat{S}_y, \hat{S}_z] = -i\hbar \hat{S}_x, \quad [\hat{S}_z, \hat{S}_x] = -i\hbar \hat{S}_y$
$[\hat{\vec{S}}^2, \hat{S}_x] = 0, \quad [\hat{\vec{S}}^2, \hat{S}_y] = 0, \quad [\hat{\vec{S}}^2, \hat{S}_z] = 0$

$\hat{S}_z \chi_{sm_s} = S_z \chi_{sm_s}$
$S_z = m_s \hbar$
$\hat{\vec{S}}^2 \chi_{sm_s} = \vec{S}^2 \chi_{sm_s}$
$\vec{S}^2 = s(s+1)\hbar^2, \quad |m_s| \leq s$
Elektron ima $s = \frac{1}{2} \implies$
$m_s = \pm\frac{1}{2}$
$\Psi_{nlm_l m_s}(r, \vartheta, \varphi, t) = R_{nl}(r) Y_{lm_l}(\vartheta, \varphi) \chi_{sm_s} e^{-iE_{nlm_l m_s} t/\hbar}$
Izven magnetnega polja je degeneracija $2n^2$ kratna.

$\hat{\vec{\mu}}_s = -g_s \mu_B \frac{\hat{\vec{S}}}{\hbar} \quad (g_s = 2)$

Seštevanje vrtilnih količin

$\vec{L} = \vec{L}_1 + \vec{L}_2$
$m = m_1 + m_2$
Za l imamo več možnosti.
$|lm\rangle = \sum_{m_1+m_2=m} C^{lm}_{l_1 m_1, l_2 m_2} |l_1 m_1, l_2 m_2\rangle$

$\vec{J} = \vec{L} + \vec{S}$
$||\vec{L}| - |\vec{S}|| \leq |\vec{J}| \leq |\vec{L}| + |\vec{S}|$
$[\hat{J}_x, \hat{J}_y] = -i\hbar \hat{J}_z, \quad [\hat{J}_y, \hat{J}_z] = -i\hbar \hat{J}_x, \quad [\hat{J}_z, \hat{J}_x] = -i\hbar \hat{J}_y$
$[\hat{\vec{J}}^2, \hat{J}_x] = 0, \quad [\hat{\vec{J}}^2, \hat{J}_y] = 0, \quad [\hat{\vec{J}}^2, \hat{J}_z] = 0$
$J_z = m_j \hbar, \quad |m_j| = -j, -j+1, \ldots j$
$\vec{J}^2 = j(j+1)\hbar^2, \quad j = l \pm \frac{1}{2}$
Vodikove VF so lahko tudi ψ_{nljm_j}
$\hat{\vec{\mu}} = \hat{\vec{\mu}}_l + \hat{\vec{\mu}}_s = -(g_l \hat{\vec{L}} + g_s \hat{\vec{S}}) \frac{\mu_B}{\hbar} = -(\hat{\vec{J}} + \hat{\vec{S}}) \frac{\mu_B}{\hbar}$

Sklopitev spin-tir (fina struktura, $B = 0$)

$\hat{H}_{ls} = Z\alpha \frac{\hbar}{2m_e^2 c} \frac{\widehat{\vec{L}\cdot\vec{S}}}{r^3}$
$\langle E_{ls} \rangle = \frac{Z^4 \alpha^2}{n^3} E_0 \frac{j(j+1) - l(l+1) - s(s+1)}{l(l+1)(2l+1)}$
Če upoštevamo sklopitev $\vec{L} \cdot \vec{S}$, moramo lastne funkcije opisovati z n, l, j, m_j.
Če upoštevamo še relativistični popravek:
$\langle E_{ls} \rangle + \langle T_{\mathrm{rel}} \rangle = -\frac{Z^4 \alpha^4}{2n^3} m_e c^2 \left(\frac{2}{j+1} - \frac{3}{4n} \right)$

Zeemanov pojav - močno magnetno polje

Zanemarimo sklopitev spin-tir.
$\langle E_{\mathrm{mag}} \rangle = \frac{\mu_B}{\hbar} \langle L_z + 2S_z \rangle B = (m_l + 2m_s) \mu_B B$

Zeemanov pojav - šibko magnetno polje

$\langle \mu_z \rangle = -g\mu_B \frac{\langle J_z \rangle}{\hbar}$
$\langle \vec{\mu} \rangle = -g\mu_B \frac{\langle \vec{J} \rangle}{\hbar}$
$g = \langle \frac{\widehat{\vec{J}^2 + \vec{L}\cdot\vec{S}}}{\hat{\vec{J}}^2} \rangle = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}$ (Lande)

Sevanje atomov

$\hat{\vec{p}}_e = e(\vec{r}^+ - \vec{r}^-)$
$\langle n | \hat{\vec{p}}_e | m \rangle = \vec{p}_{e_{nm}}(t) = e^{-i(E_m - E_n)t/\hbar} \vec{p}_{e_{nm}}$
$\vec{p}_{e_{nm}}, \vec{p}_{e_{mn}} \in \mathbb{R} \implies \vec{p}_{e_{nm}} = \vec{p}_{e_{mn}} = \int \psi_n \hat{\vec{p}}_e \psi_m \, dV$

$\Psi_\alpha = c_1(t)\Psi_1 + c_2(t)\Psi_2 \quad$ (prehod $2 \to 1$)
$\langle \alpha | \hat{\vec{p}}_e | \alpha \rangle =$
$= c_1^2 \langle 1 | \hat{\vec{p}}_e | 1 \rangle + c_2^2 \langle 2 | \hat{\vec{p}}_e | 2 \rangle + c_1 c_2 (\langle 1 | \hat{\vec{p}}_e | 2 \rangle + \langle 2 | \hat{\vec{p}}_e | 1 \rangle) =$
$= 2c_1 c_2 \vec{p}_{e_{12}} \cos \omega_{12} t$
$\omega_{12} = \frac{E_2 - E_1}{\hbar}$
$c_2^2(t) = c_2^2(0) e^{-t/\tau}$
$\frac{1}{\tau} = \frac{\omega_{12}^3 \vec{p}_{e_{12}}^2}{3\pi\varepsilon_0 c^3 \hbar}$
$P = \frac{\hbar\omega_{12}}{\tau} = \frac{\omega_{12}^4 \vec{p}_{e_{12}}^2}{3\pi\varepsilon_0 c^3}$

Izbirna pravila

Prehod $n \to m$ je dovoljen, če $\vec{p}_{e_{mn}} \neq 0$ (matrični element).

Neskončna potencialna jama:
Prehod $n_2 \to n_1$ dovoljen, če je en n sod, drugi lih.

Vodikov atom:
$\Delta l = \pm 1 \quad \Delta m_l = 0, \pm 1, \quad \Delta m_s = 0, \quad \Delta s = 0$
Upoštevajoč sklopitev spin-tir:
$\Delta l = \pm 1 \quad \Delta j = 0, \pm 1, \quad \Delta m_j = 0, \pm 1, \quad \Delta s = 0$

Rotator: $\Delta l = \pm 1$
Harmonični oscilator: $\Delta n = \pm 1$

Foton ima $s = 1, m_s = \pm 1$. Ne more imeti $m_s = 0$, saj bi to ustrezalo longitudinalnemu valovanju.

Širina spektralnih črt

$E_{1/2} \tau = \hbar \quad$ (FWHM)
$\omega_{1/2} = \frac{W_{1/2}}{\hbar} = \frac{1}{\tau}$
$\nu_{1/2} = \frac{1}{2\pi\tau}, \qquad \lambda_{1/2} = \frac{\lambda^2}{2\pi\tau c}$
$\delta\omega_D = \sqrt{\frac{k_B T}{m_1 c^2}} \omega_0 \quad$ (Doppler)
$\delta\omega_c = \frac{1}{\tau_c} = \frac{\langle v \rangle}{\langle l \rangle} = 2\sqrt{\frac{2\pi}{m k_B T}} (2r_1)^2 p \quad$ (trki)

Večelektronski atom

$V = -\sum_{i=1}^{Z} \frac{Ze^2}{4\pi\varepsilon_0 |\vec{r}_i|} + \sum_{i<j}^{Z} \frac{e^2}{4\pi\varepsilon_0 |\vec{r}_i - \vec{r}_j|}$

Približek golega jedra

$V = \sum_{i=1}^{Z} \frac{Ze^2}{4\pi\varepsilon_0 |\vec{r}_i|}$
$E = \sum_i E_i$
Senčenje: $V_C(r) = -\frac{e^2}{4\pi\varepsilon_0 |\vec{r}_i|} Z_{\mathrm{ef}}(r)$

Paulijeva prepoved

Posamezni e^- morajo biti v enodelčnih stanjih, ki se med seboj razlikujejo vsaj po enem kvantnem številu.
Večdelčna VF mora biti antisimetrična:

$$\psi(\vec{r}_1, \ldots, \vec{r}_Z) = \frac{1}{\sqrt{(Z!)}} \begin{vmatrix} \psi_1(\vec{r}_1) & \psi_1(\vec{r}_2) & \cdots & \psi_1(\vec{r}_Z) \\ \psi_2(\vec{r}_1) & \psi_2(\vec{r}_2) & \cdots & \psi_2(\vec{r}_Z) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_Z(\vec{r}_1) & \psi_Z(\vec{r}_2) & \cdots & \psi_Z(\vec{r}_Z) \end{vmatrix}$$

Rentgenski spekter

$\frac{1}{\lambda_{K_\alpha}} = \frac{(Z-1)^2}{\lambda_0}$
$j = j_0 e^{-\mu x}$
$\frac{1}{\lambda_{\text{rob K}}} = \frac{(Z-1)^2}{\tilde{\lambda}_0}$

Molekule

$E_\pm = E_{1s} + G \pm S$
Vez H-H (A - kovalentni del, B, C - ionski del): $\psi(1,2) =$
$\{A \frac{1}{\sqrt{2}} \left[\Phi_{1s}(\vec{r}_1 - \frac{\vec{R}}{2}) \Phi_{1s}(\vec{r}_2 + \frac{\vec{R}}{2}) + \Phi_{1s}(\vec{r}_2 - \frac{\vec{R}}{2}) \Phi_{1s}(\vec{r}_1 + \frac{\vec{R}}{2}) \right] +$
$B \Phi_{1s}(\vec{r}_1 - \frac{\vec{R}}{2}) \Phi_{1s}(\vec{r}_2 - \frac{\vec{R}}{2}) + C \Phi_{1s}(\vec{r}_1 + \frac{\vec{R}}{2} \Phi_{1s}(\vec{r}_2 + \frac{\vec{R}}{2}))\}$

$\vec{\mathcal{E}}_d = \frac{p}{4\pi\varepsilon_0 R^3}$
$\vec{p}_2 = \alpha \vec{\mathcal{E}}_d$
$V = -\vec{p}_2 \cdot \vec{\mathcal{E}}_d \propto \frac{1}{R^6} \quad \Longrightarrow \quad F(R) \propto \frac{1}{R^7}$
$\alpha \propto V_{\mathrm{sistema}}$ (volumen)
$V_{LJ} = 4\epsilon \left[\left(\frac{\sigma}{R}\right)^n - \left(\frac{\sigma}{R}\right)^6 \right] \quad$ (Lennard-Jones)

Vzbujena stanja molekul

Rotacija: $E_{\mathrm{rot}} = \frac{\hbar l(l+1)}{2\mu R_0^2}$
$\frac{\hbar^2}{2\mu R_0^2} \approx 7 \cdot 10^{-3}$eV za H_2
Vibracija: $E_{\mathrm{vib}} = \hbar\omega_0(\frac{1}{2} + n)$
$\hbar\omega_0 = \hbar\sqrt{\frac{k}{\mu}} \approx 0{,}2$eV za O_2

Čisti rotacijski prehod: $\Delta l = \pm 1$.
Vibracijsko – rotacijski prehod: $\Delta n = \pm 1, \Delta l = \pm 1$.
Elektronski prehod: ni zahteve.

$n(l) = (2l+1) \exp\{ \left[\frac{1}{2}\hbar\omega_0 + Bl(l+1) \right] / k_b T \}$
$B = \frac{\hbar^2}{2\mu R_0^2} \neq const.$, saj $R_0 \neq const.$

Fizikalne konstante

$R = 8\ 310\ \frac{\mathrm{J}}{\mathrm{kmol\ K}}$
$N_A = 6{,}02 \cdot 10^{26}\ \frac{1}{\mathrm{kmol}}$
$k_B = \frac{R}{N_A} = 1{,}38 \cdot 10^{-23}\ \frac{\mathrm{J}}{\mathrm{K}}$

$e_0 = 1{,}602 \cdot 10^{-19}$ As
$\varepsilon_0 = 8{,}85 \cdot 10^{-12}\ \frac{\mathrm{As}}{\mathrm{Vm}}$
$\mu_0 = 4\pi \cdot 10^{-7}\ \frac{\mathrm{Vs}}{\mathrm{Am}}$
$c_0 = 3{,}0 \cdot 10^8\ \frac{\mathrm{m}}{\mathrm{s}}$
$\sigma = 5{,}67 \cdot 10^{-8}\ \frac{\mathrm{W}}{\mathrm{m^2 K^4}}$
$k_W = 2{,}90 \cdot 10^{-3}\ \mathrm{m \cdot K}$

$u = 1{,}66 \cdot 10^{-27}\ \mathrm{kg} = 931{,}5\ \frac{\mathrm{MeV}}{\mathrm{c^2}}$
$m_e = 9{,}1 \cdot 10^{-31}\ \mathrm{kg} = 0{,}511\ \frac{\mathrm{MeV}}{\mathrm{c^2}}$
$m_p = 1{,}673 \cdot 10^{-27}\ \mathrm{kg} = 938{,}3\ \frac{\mathrm{MeV}}{\mathrm{c^2}} = 1{,}00728u$
$m_n = 1{,}675 \cdot 10^{-27}\ \mathrm{kg} = 939{,}6\ \frac{\mathrm{MeV}}{\mathrm{c^2}} = 1{,}00866u$

$h = 6{,}626 \cdot 10^{-34}$ Js
$hc = 1240$ eV nm
$r_B = 5{,}291 \cdot 10^{-2}$ nm
$E_0 = 13{,}6$ eV
$\lambda_c = 2{,}426 \cdot 10^{-3}$ nm
$\mu_B = \frac{e_0\hbar}{2m_e} = 5{,}79 \cdot 10^{-5}\ \frac{\mathrm{eV}}{\mathrm{T}}$
$\alpha = \frac{e_0^2}{4\pi\varepsilon_0\hbar c} = \frac{1}{137}$
$\lambda_0 = \frac{4hc}{3E_0} = 121{,}6$ nm
$\tilde{\lambda}_0 = \frac{hc}{E_0} = 91{,}2$ nm