

$$\vec{L}^2 = \vec{L} \cdot \vec{L} = (\vec{r} \times \vec{p}) \cdot (\vec{r} \times \vec{p}) = L_x^2 + L_y^2 + L_z^2 = L^2$$

• Lastnosti

$$\bullet \underline{[L_\alpha, L_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} L_\gamma}$$

$$[X_\alpha, P_\beta] = i\hbar \delta_{\alpha\beta}$$

$$[X_\alpha, X_\beta] = 0$$

$$[P_\alpha, P_\beta] = 0$$

$$\underline{[L_x, L_y]} = [y p_z - z p_y, z p_x - x p_z] =$$

$$= [y p_z, z p_x] - [p_y z, z p_x] - [y p_z, x p_z] + [p_y z, x p_z] =$$

$$= y p_x [p_z, z] + x p_y [z, p_z] = i\hbar (x p_y - y p_x) = \underline{\underline{i\hbar L_z}}$$

$$\bullet \bullet [L_\alpha, A_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} A_\gamma; \quad \vec{A} = \vec{r}, \vec{p}, \vec{L}, \dots$$

$\bullet \bullet$   $\vec{L}$  komutirajoči operatorji

$$[\vec{L}, \hat{A}] = 0$$

$$u(\vec{r}) \hat{A} = \hat{A} u(\vec{r})$$

neku op.  $\uparrow$

$$a) \hat{A} = c \in \mathbb{C} \text{ konstanta } \checkmark$$

$$b) \hat{A} = \vec{r} \cdot \vec{r} = r^2 = |\vec{r}|^2 \checkmark$$

$$\vec{p} \cdot \vec{p} = p^2 \checkmark$$

$$\underline{\vec{L} \cdot \vec{L}} = L^2 \checkmark \Rightarrow [L_\alpha, L^2] = 0$$

$$\Rightarrow [L^2, H] = 0$$

$$\text{če } L \rangle H = \frac{p^2}{2m} + V(|\vec{r}|)$$

abs. vrednost



∴ Lestvični operatorji (ladder operator)

$$L_{\pm} = L_x \pm iL_y = (L_{\mp})^{\dagger}$$

↔  
"ustreza"

$$[L^2, L_{\pm}] = 0$$

$$L_z \sim \hat{n}$$

$$a \sim L_{-}$$

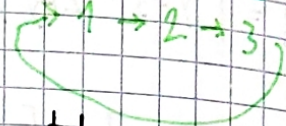
$$a^{\dagger} \sim L_{+}$$

$$[n, a^{\dagger}] = a^{\dagger}$$

$$[n, a] = -a$$

$$L_z \sim \hat{n}$$

$$x \rightarrow y \rightarrow z$$



$$1) [L_z, L_{+}] = [L_z, L_x + iL_y] =$$

$$= [L_z, L_x] + i[L_z, L_y] =$$

$$= i\hbar L_y + (-i)\hbar L_x = \hbar L_x + i\hbar L_y = \hbar L_{+}$$

$$\Rightarrow [L_z, L_{\pm}] = \pm \hbar L_{\pm}$$

$$2) L_{+}L_{-} = (L_x + iL_y)(L_x - iL_y) = L_x^2 + L_y^2 + iL_yL_x - iL_xL_y = L^2 - L_z^2$$

$$= L^2 + \hbar L_z - L_z^2$$

$$\Rightarrow L_{\pm}L_{\mp} = L^2 \pm \hbar L_z - L_z^2$$

$$[L_{+}, L_{-}] = 2\hbar L_z$$

↔  
ustreza

$$[a, a^{\dagger}] = 1$$

^ Lastne vrednosti  $L_z, L^2$

$$L_z |m\rangle = m\hbar |m\rangle; \quad m \in \mathbb{R}$$

To bi lahko rešili običajno:

$$-i\hbar \frac{\partial}{\partial \varphi} = L_z$$

$$-i\hbar \frac{\partial}{\partial \varphi} \psi_m(\varphi) = m\hbar \psi_m(\varphi) \Rightarrow \psi_m = C_m e^{im\varphi}$$



Raje naredimo kot pri LHO z  $a$  in  $a^\dagger$ :

$$L_z L_\pm |m\rangle = (L_z L_\pm \pm \hbar L_\pm) |m\rangle = (m \pm 1) \hbar L_\pm |m\rangle = \alpha |m \pm 1\rangle$$

$L_+$  in  $L_-$  tvorj  
zvišujeta ali znižujeta  
lastno vrednost.

$$\therefore [L^2, L_z] = 0$$

$$L^2 |m\rangle = \lambda |m\rangle; \quad \lambda \in \mathbb{R} \text{ ker je } L^2 \text{ hermitski}$$

$$\langle m | L^2 |m\rangle = \langle m | \sum_{\alpha} L_{\alpha}^2 |m\rangle = \sum_{\alpha} \langle L_{\alpha} m | L_{\alpha} m \rangle \geq 0$$

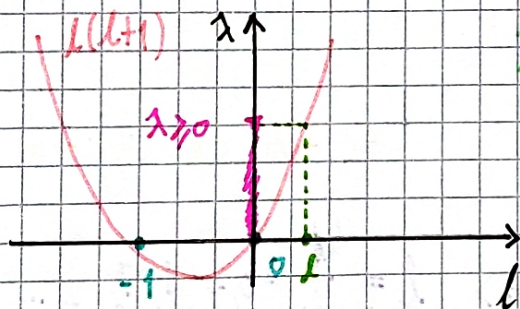
↑ Ker je to pravzaprav norma  
vektorja

$$m = \lambda \langle m | m \rangle \geq 0$$

$\Rightarrow \lambda \geq 0$  Operator  $L^2$  je semipozitivno definiten

$$L^2 L_\pm |m\rangle = L_\pm L^2 |m\rangle = \lambda L_\pm |m\rangle$$

$$\lambda = l(l+1)\hbar^2$$



$\lambda \leftrightarrow l \geq 0$   
bijektivno

~~$L^2 |l, m\rangle$~~

$$L^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle$$

$$L_z |l, m\rangle = m\hbar |l, m\rangle$$

$$\langle L_+ \Psi_{lm} | L_+ \Psi_{lm} \rangle = \langle \Psi_{lm} | (L_+)^{\dagger} L_+ | \Psi_{lm} \rangle = \langle \Psi_{lm} | L_- L_+ | \Psi_{lm} \rangle \geq 0$$

$$\langle l, m | L_- L_+ | l, m \rangle = \langle l, m | (L^2 - L_z^2 - \hbar L_z) | l, m \rangle =$$

$$= \underbrace{(l(l+1)\hbar^2 - m(m \pm 1)\hbar^2)}_{\geq 0} \langle l, m | l, m \rangle \geq 0$$



$$\text{če } m \geq 0; l \geq 0: m(m+1) \leq l(l+1) \Rightarrow m \leq l$$

$$m \leq 0; l \geq 0: \Rightarrow -m \geq -l$$

$$\Rightarrow \underline{|m| \leq l}$$

$$\underline{L_{\pm} |lm\rangle = \hbar \sqrt{l(l+1) - m(m\pm 1)} |l, m\pm 1\rangle}$$

$$|l, m\pm 1\rangle = \frac{1}{\hbar \sqrt{l(l+1) - m(m\pm 1)}} L_{\pm} |lm\rangle$$

Vzamemo največji m možen:

$$L_- |ll\rangle = C_{l,l-1} |l, l-1\rangle$$

$$L_- L_- |ll\rangle = C_{l,l-2} |l, l-2\rangle$$

⋮

$$L_-^k |ll\rangle = C_{l,l-k} |l, l-k\rangle$$

Tolikokrat da je  $-l$

$$l-k=l \Rightarrow 2l=k \Rightarrow l = \frac{k}{2} = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$$

S tem smo ugotovili kaksni so  $l$

Torej smo ugotovili:

$$L_z |lm\rangle = m\hbar |lm\rangle$$

$$L^2 |lm\rangle = l(l+1)\hbar^2 |lm\rangle$$

$$l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$$

$$|m| \leq l$$



Zakaj so rešitve  $l$  za Vodnikov atom samo celostneštke?

$$l = 0, 1, 2, \dots$$

$m \dots$

$$\psi_{lm} = C e^{im\phi}$$

Vodikova VF

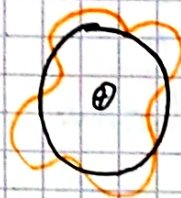
$$H\psi(\vec{r}) = E\psi(\vec{r})$$

Zvezna

$$L_z \psi = m\hbar \psi$$

$$e^{im(\phi+2\pi)} = e^{im\phi}$$

Bohr:



Kvantiziral vrtilno količino

Če hočemo zvezno

$$m \in \mathbb{Z}$$

$\Leftarrow$

$$e^{im2\pi} = 1$$

Rešitve (funkcije)

Rešitve so sferični harmoniki.

$$Y_l^m(\theta, \phi); \quad \langle r | l m \rangle = \psi(r) Y_l^m$$

Sferični harmoniki:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{4\pi}} \sin\theta e^{i\phi}$$

To so tisti "mehurčki", ki predstavljajo orbitale

Tudi bomo realni

$$Y_{lm} \quad \begin{matrix} \cos\phi \\ \cos m\phi \end{matrix} \text{ namesto } e^{im\phi}$$

Orbitale: s, p, d, f, ... (ne j)

$p_x, d_{xy}, d_{z^2}$

To so trije načini

Zapis operatorja  $L$  z matriko

$$|\psi\rangle = \sum_{l=0}^{\infty} \sum_{m=-l}^l C_{lm} |lm\rangle$$

Splošno:

$$L_+ = \sum_{n n'} |n\rangle \langle n| L |n'\rangle \langle n'|$$

Pri nas:

$$= \sum_{\substack{l l' \\ m m'}} |l' m'\rangle (L_+)_{l' m', l m} \langle l m|$$



$$(L_+)_m^m = \langle l' m' | L_+ | l m \rangle =$$

↳ Matrica matricnih elementov

ortogonalnost

$$= \langle l' m' | \hbar \sqrt{l(l+1) - m(m+1)} | l, m+1 \rangle \delta_{l'l} \delta_{m', m+1}$$

$$L_+ |l, m\rangle \rightarrow \begin{pmatrix} 0 & & & & & & \dots \\ \hline \underbrace{0 \quad \sqrt{2} \quad 0}_{l=0} & & & & & & \dots \\ & 0 \quad 0 \quad \sqrt{2} & & & & & \dots \\ \hline \underbrace{0 \quad 0 \quad 0}_{l=1} & & & & & & \dots \\ & 0 \quad \sqrt{4} \quad 0 \quad 0 \quad 0 & & & & & \dots \\ & 0 \quad 0 \quad \sqrt{6} \quad 0 \quad 0 & & & & & \dots \\ & 0 \quad 0 \quad 0 \quad \sqrt{6} \quad 0 & & & & & \dots \\ & 0 \quad 0 \quad 0 \quad 0 \quad \sqrt{4} & & & & & \dots \\ & 0 \quad 0 \quad 0 \quad 0 \quad 0 & & & & & \dots \\ & \vdots & & & & & \dots \\ & \vdots & & & & & \dots \end{pmatrix} \begin{pmatrix} C_{00} \\ C_{11} \\ C_{10} \\ C_{1-1} \\ \hline C_{22} \\ C_{21} \\ C_{20} \\ C_{2-1} \\ C_{2,-2} \\ \vdots \\ \vdots \end{pmatrix}$$

Ramšal ne more  
 $|l, m\rangle \propto \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$   
 Ampak je to sicer n  
 kveji ima  
 $\psi = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$   
 da ne enačiš bet s  
 stolpcem.

DN

$l=1$

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$L_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$L_z = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Izračeni v lastni bazi  $L_z$

→ Diagonalna sereda



# Centralni potencial $V(r)$

1)  $H = \frac{p^2}{2m} + V(r)$  invariantna na rotacije v prostoru

$$[H, \vec{L}] = 0 \quad \vec{r} \cdot \vec{L} = 0$$

$$[H, L^2] = 0 \quad \vec{p} \cdot \vec{L} = 0$$

$$\nabla^2 = \Delta = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + (\theta, \phi) \quad \text{v kolinarnih}$$

$$H = -\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right) + \frac{L^2}{2mr^2}$$

To nam omogoči, da zapišemo:  $\Psi(r, \theta, \phi) = \psi(r) Y_{\ell}^m(\theta, \phi)$

$$H\Psi = E\Psi \quad \text{Veff}(r)$$

$$\Rightarrow \left[ -\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right) + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r) \right] \Psi(r, \theta, \phi) = E\Psi(r, \theta, \phi)$$

Nastavek za  $\Psi(r)$ :

$$\Psi(r) = \frac{u(r)}{r} \quad \text{v 3D} \quad \nabla$$

$$\left( \begin{array}{l} \Psi(r) = \frac{u(r)}{r} \quad \text{v 2D} \\ \Psi(r) = u(r) \quad \text{v 1D} \end{array} \right)$$

Uporabimo nastavek:

$$\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \frac{u}{r} = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \left( \frac{u'}{r} - \frac{u}{r^2} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} (ru' - u) = \frac{u''}{r} = \frac{1}{r} \frac{\partial^2 u}{\partial r^2}$$

Torej se operator poenostavi v tem primeru.

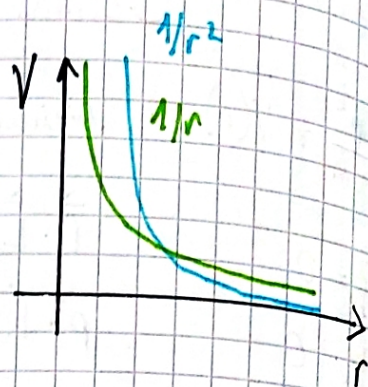
$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right] u(r) = E u(r);$$

$$V_{\text{eff}} = V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}$$



# Lastnosti rešitev

a)  $\hbar \rightarrow 0$ : Omejimo na primerke  $\lim_{r \rightarrow 0} r^2 V(r) = 0$



$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} = \frac{l(l+1)\hbar^2}{2mr^2} u; \quad u = Cr^\lambda$$

$$\lambda(\lambda-1) = l(l+1) \Rightarrow \lambda_{1,2} = l+1, -l$$

$$u(r) = C_1 r^{l+1} + D_1 \frac{1}{r^l}$$

$$l > 0: \langle \Psi, \Psi \rangle = \int |Y_l^m|^2 d\Omega \int_0^\infty |\Psi|^2 r^2 dr \stackrel{=1}{=} C_1 < \infty$$

$\Rightarrow D_L = 0$ ; Sicer se ne da normirati

$$l=0: u = C_0 r + D$$

$$\int_0^\infty |\Psi|^2 r^2 dr \xrightarrow{r \rightarrow 0} \frac{|D_0|^2}{r^2} r^2 = |D_0|^2 \sqrt{??}$$

V elektrostatiiki:

$$f = \frac{C_1}{r} = \frac{e}{4\pi\epsilon_0 r}$$

$$\nabla^2 \phi = \lambda \delta(r)$$

$$\Rightarrow D_0 = 0$$

Rešitev je:  $\Psi = C_l r^l = \frac{C_l r^{l+1}}{r}$

b)  $r \rightarrow \infty$ :

•  $E > 0$ :

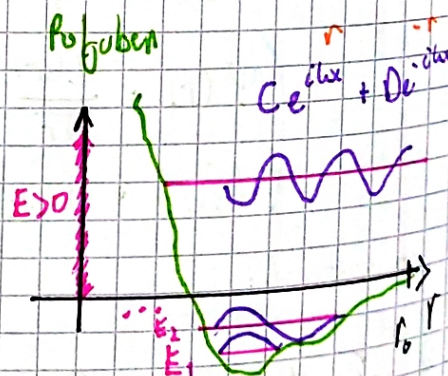
Predpostavimo  $V \rightarrow$  dovolj hitro

$$V = 0 \quad \text{za} \quad r > r_0$$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} = E u$$

$$u(r) = C_+ e^{i\sqrt{k}r} + C_- e^{-i\sqrt{k}r}$$

$$E_a = \frac{\hbar^2 k^2}{2m}$$





..  $E < 0$

$$u(r) = D_+ e^{\alpha r} + D_- e^{-\alpha r} \quad E_n = -\frac{\hbar^2 \alpha^2}{2m}$$

$\rightarrow D_+ = 0$ , da jo lahko normiramo

Takeaway:

$$u(r) = r^{l+1} v(r) e^{-\alpha r}$$

↑  
majhne  
razdalje

↓  
ker je vmes  
(konst za  $r \rightarrow 0$  in  $r \rightarrow \infty$ )

← velike razdalje

### Coulombski potencial

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} - \frac{e_0^2}{4\pi\epsilon_0 r} \right) u = E u$$

$$\Psi(\vec{r}) = \frac{u(r)}{r} Y_l^m(\theta, \phi) \quad g = \alpha r, \quad |E| = \frac{\alpha^2 \hbar^2}{2m}$$

Enačbo pomnožimo z  $\frac{2m}{\hbar^2 \alpha^2}$  in dobimo:

Wec le parameter

$$\left( -\frac{d^2}{dg^2} + \frac{l(l+1)}{g^2} + \frac{g_0}{g} - 1 \right) u = 0; \quad g_0 = \frac{m e_0^2}{2\pi \epsilon_0 \hbar^2 \alpha}$$

$$u(g) \leftarrow u(r(g))$$

Za majhne razdalje smo pokazali  $u(g) = g^{l+1}$

Za velike razdalje pa  $u(r) \rightarrow e^{-g}$

$$\Rightarrow u(g) = g^{l+1} v(g) e^{-g}$$

↓  
↓

$$u''(g) = \dots v'' \dots v' \dots v$$

Vstavimo in poračunamo.



Dobimo:

$$g v'' + 2(l+1-g)v' + (g_0 - 2(l+1))v = 0$$

To se rešuje z razvojem v vrsto (kot pri mat 4)

$$v(g) = \sum_{h=0}^{\infty} c_h g^h$$

$$v'(g) = \sum_{h=0}^{\infty} h c_h g^{h-1} \rightarrow v' = \sum_{h=0}^{\infty} (h+1) c_{h+1} g^h$$

$$v''(g) = \sum_{h=0}^{\infty} h(h+1) c_{h+1} g^{h-1}$$

To vstavimo:

$$\sum_{h=0}^{\infty} g^h \left( [h(h+1) + 2(l+1)(h+1)] c_{h+1} + [-2h + (g_0 - 2(l+1))] c_h \right) = 0$$

$$\rightarrow c_{h+1} = \frac{2(l+1) - g_0}{(h+1)(h+2(l+1))} c_h$$

Pogledajmo  $h \gg 1$ :

$$c_{h+1} = \frac{2l}{h^2} c_h = \frac{2}{h} c_h$$

$$e^{2x} = \sum_{h=0}^{\infty} \frac{2^h x^h}{h!}$$

$$\frac{2^{h+1} h!}{(h+1)! 2^h} \rightarrow \frac{2}{h}$$

Kar smo ugotovili:

$$u(g) \rightarrow e^{2g} \quad (g \rightarrow \infty, h \rightarrow \infty)$$

$$\Rightarrow u(g) \Rightarrow g^{l+1} e^{2g} e^{-g} = g^{l+1} e^g$$



$$\exists l_{\max} : 2(l+1) - l_0 = 0$$

$$C_{l_{\max}+1} = 0$$

Sistem omajimo vrsto na polinom reda  $l_{\max}$ :

$$\sum_{l=0}^{l_{\max}} C_l r^l = V(r) ; l = 0, 1, 2, \dots, l_{\max} ; n = l_{\max} + l + 1 \geq 1$$

$$l_0 = 2n = 2, 4, 6, \dots$$

$$E = -\frac{\hbar^2}{2m} = -\frac{me^2}{8\pi^2 \epsilon_0^2 \hbar^2 a_0^2}$$

In dobimo to kar je Bohr dobil:

$$|E_1| = 1R_y = 13.6 \text{ eV}$$

Rydbergova konstanta

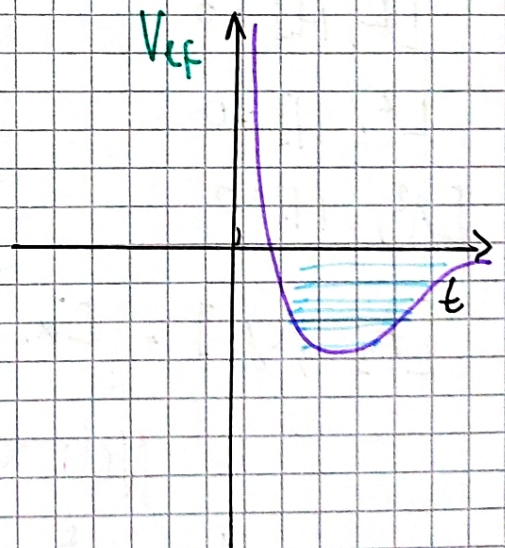
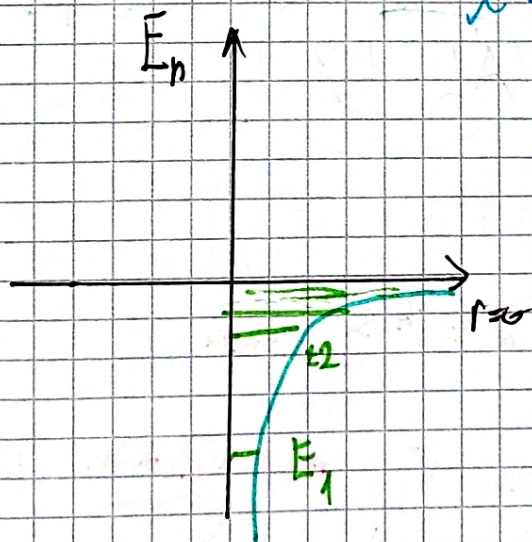
$$E_n = -\frac{M}{2\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \frac{1}{n^2} = -\frac{|E_1|}{n^2}$$

Degeneracija

$$E_n = \frac{1R_y}{n^2} ; n = l+1, 2, \dots$$

$$l = 0, 1, 2, \dots$$

| n | l | l |
|---|---|---|
| 1 | 0 | 0 |
| 2 | 1 | 0 |
| 2 | 0 | 1 |
| 3 | 2 | 0 |
| 3 | 1 | 1 |
| 3 | 0 | 2 |
| ⋮ | ⋮ | ⋮ |



$$l = 0, 1, \dots, n-1$$

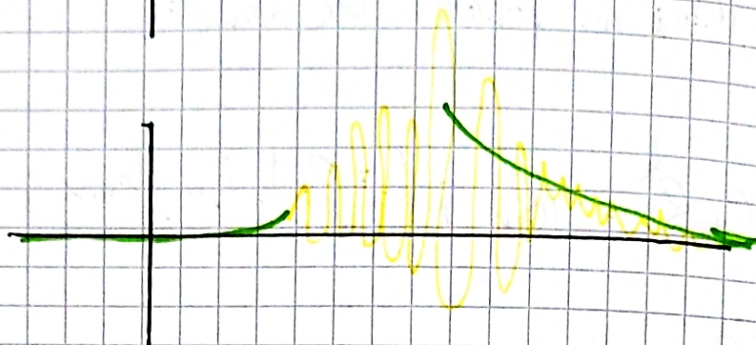
$$m_l = -l, -l+1, \dots, l$$

$$2l+1$$



klasična rešitev

$$n \gg 1$$



Primer:

$$\sigma = \frac{n(n+1)}{2^2}$$

$$r = 1 \text{ cm}$$

$$F = 100 \text{ 000 V}$$

$$n \sim 10^{36}$$

Kvantni: Laplace - Lenzov vektor

$$\vec{A} = \frac{1}{2} \left[ \vec{p} \times \vec{r} + (\vec{p} \times \vec{L}) \right] - \frac{mc^2}{4\pi\epsilon_0} \frac{\vec{r}}{r} - (\vec{L} \times \vec{p})$$

$$[L, H] = 0$$

$$[L^2, H] = 0$$

$$[A^2, H] = 0$$

$$\vec{A} \cdot \vec{L} = L_x$$

$$[A_x, A_y] = [A_x, A_z] = [A_y, A_z] = i\hbar A_z$$

Neli delce v magnetnem polju ( $B = \text{const}$ )

$$m\vec{a} = e\vec{E} + e\vec{v} \times \vec{B}$$

$$H = \frac{(\vec{p} - e\vec{A})^2}{2m} + \phi_e$$



Veľjia

$$\vec{B} = \nabla \times \vec{A}$$

$$\vec{E} = -\nabla\phi - \frac{\partial}{\partial t} \vec{A}$$

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m} (-i\hbar \nabla - e\vec{A})^2 \psi + e\phi \psi$$

$$(\nabla \vec{A}) \psi + (\vec{A} \cdot \nabla) \psi - \nabla \vec{A} \psi - \hat{A} \nabla \psi -$$

$$- 2\vec{A} \nabla \psi + \psi \nabla \vec{A}$$

$$i \frac{\hbar \partial \psi}{\partial t} = \frac{-\hbar^2 \nabla^2}{2m} \psi + \underbrace{i \frac{\hbar e}{m} \vec{A} \cdot \nabla \psi}_{\text{Zeeman}} + \left( \frac{i\hbar e}{m} (\nabla \cdot \vec{A}) + \frac{e^2 A^2}{2m} e\phi \right) \psi$$

Coulombovona potencie vrste

Zamenjiva sklopiter

$$\nabla = 0, \vec{A} = \frac{1}{2} (\vec{r} \times \vec{B})$$

$$\frac{i\hbar e}{m} \vec{A} \cdot \nabla \psi = - \frac{i\hbar}{2m} (\vec{r} \times \vec{B}) \cdot \nabla \psi =$$

$$= \frac{\hbar}{2m} \dots = i \frac{\hbar e}{2m} ((\vec{r} \times \vec{B}) \cdot \nabla \psi) =$$

$$= \frac{q}{2m} (\vec{r} \times \vec{p}) \cdot \vec{B} \psi = - \frac{e}{2m} \vec{B} \cdot \vec{L} \psi$$

$$\text{Heisenberg} = -\vec{\mu} \cdot \vec{B} \rightarrow \vec{\mu} = 2 \frac{e}{m} \vec{L}$$

$$\text{Heisenberg} = -\mu \vec{B}; \quad \vec{\mu} = \frac{e}{2m} \vec{L}$$

$$\dots \frac{e^2}{2m} \vec{A} \cdot \vec{A} \frac{dB^2}{B^2} (x^2 + y^2) \psi; \quad \psi \Rightarrow A, \frac{B}{2} (-y, x, 0) \psi$$

and  $(L_z = \frac{\hbar}{2m} L)$



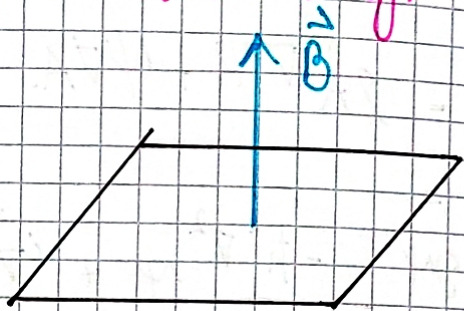
$B = 10 \text{ Tm}$   
 $x_2 \sim 10 \text{ nm}$

$\frac{H_2}{H} \sim \frac{b}{\text{miles}}$   
 $\sim 10$

Homogeno magnetno polje: Landauovi nivoji

$\vec{B} = B e_z$

$\vec{A} = -\frac{1}{2}(\vec{r} \times \vec{B}) = \frac{B}{2}(-y, x, 0)$



$\vec{A} = B(-y, 0, 0)$  } Landauova umetitev

ali  
 $\vec{A} = B(0, x, 0)$

$\vec{B} = \nabla \times \vec{A} = (0, 0, B)$  ne  $\exists \vec{A}$ , ki ima simetrije problema

$\frac{1}{2m} \left[ (-i\hbar \frac{\partial}{\partial x} + eBy) \right]^2 - \frac{\hbar^2 \partial^2}{2m} - \hbar^2 \frac{\partial^2}{2m z^2} \psi + e\phi \psi = E\psi$

$\psi(\vec{r}) = e^{i(\frac{p_x}{\hbar} x + \frac{p_z}{\hbar} z)} \chi(y) ; \phi = \phi(z)$   
 $= 0$

$\hat{A} = (1, 2, 5, \text{Pog})$



$\hat{A}: f(\hat{A}) \psi_a = f(a) \psi_a$

$\hat{A} \psi, \hat{A} \psi$  (out)



Obtane  

$$\left( \hat{p}_x - i\hbar \frac{\partial}{\partial x} \right) e^{i \frac{p_x x}{\hbar}} = f(p_x) \exp \frac{i}{\hbar} (\hat{p}_x + eB_y) x^2$$

$$\frac{1}{2m} [\hat{p}_x + eB_y] - \left[ \frac{2\omega \hbar^2}{4m\omega \hbar} \text{off} \right] \quad V(y) = E\lambda$$

$$V(y) = e\phi(y) + \frac{p_x^2}{2m} \Rightarrow \text{Lagrange multiplier LHO.}$$

$$V=0 \quad \omega = \frac{eB}{m}; \quad \frac{E}{\hbar} = \sqrt{\frac{\hbar}{eB}}; \quad p_x = \hbar k; \quad y_k = -\beta^2 k = -\frac{\hbar}{eB} k$$

$$\Rightarrow \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + \frac{1}{2} m \omega^2 (y - y_k)^2 \right] \chi_m = E_m \chi_m$$
  

$$E_n = \frac{1}{2} (\omega \hbar + \frac{1}{2})$$

$$\Rightarrow E_{nm}(x, y) (x_i) = \frac{1}{\sqrt{2\pi}} e^{ikx} \frac{1}{\sqrt{\text{index}}}$$
  

$$p_m (y - y_k)$$

$$\psi(x, t) = \int \tilde{\psi} \frac{e}{\sqrt{2\pi}} dk \frac{e^{-iEt}}{\hbar}$$

Typisch bei:

$$\psi(x, t) = \int_{-\infty}^{\infty} \tilde{\psi}$$

Landauauv nivu

$$E_n = \hbar \omega (n + \frac{1}{2}) \neq E_m$$

$\psi(-\infty, \infty) \neq 0$

$$\psi(x, y) = \psi(x, 0) = \int_{-\infty}^{\infty} \frac{\tilde{\psi}(k)}{\sqrt{2\pi}} e^{ikx} dk$$

$$\psi(x, t) = \int \tilde{\psi}(k) \frac{e^{i(kx - Et)}}{\sqrt{2\pi}} dk \quad E(b)$$

$$E = \hbar \omega (k + \frac{1}{2}) \neq \text{Vollkomme}$$

$$\psi(x, t) = \int \tilde{\psi}(k) \frac{e^{i(kx - Et)}}{\sqrt{2\pi \hbar \lambda}} dk$$



$$H = \hbar\omega(a^\dagger a + \frac{1}{2}) ; \quad H = \frac{(\hat{p} - e\hat{A})^2}{2m} \quad \text{lyer } \alpha \quad \vec{B} = \vec{B}_0$$

↑ To je pa splošno

$$E_n = \hbar\omega(n + \frac{1}{2})$$

$$\vec{A}_1 = B_0(-y, 0, 0)$$

$$\vec{A}_2 = B_0(0, x, 0)$$

$$\vec{A}_3 = \frac{1}{2} B_0(-y, x, 0) = \frac{1}{2} \vec{r} \times \vec{B}_0$$

Lokalne umetivene transformacije

$$\vec{B} = \nabla \times \vec{A}$$

$$\vec{E} = -\nabla \phi$$

$$\vec{A}' = \vec{A} + \nabla \Lambda ; \quad \vec{B}' = \vec{B}$$

$$\phi' = \phi - \frac{\partial}{\partial t} \Lambda ; \quad \vec{E}' = \vec{E}$$

Klasično:

$$\vec{F} = e\vec{E} + e\vec{v} \times \vec{B}$$

Resitev je neodvisna od

$$\vec{A}$$

Vemo že, da valovnim funkcijam lahko naredimo:

$$\psi_i \rightarrow e^{i\sigma} \psi_i ; \quad \sigma \in \mathbb{R}$$

se bo ravnno pokrvalal  $\rightarrow \langle \psi_i | \hat{\sigma} | \psi_j \rangle = \hat{\sigma}_{ij}$

Kako se bo spremenil  $\psi$  pri taki zamenjavi  $\vec{A}'$ ? ( $\psi \rightarrow \psi'$ )

$$\Psi'(\vec{r}, t) = e^{i\sigma(\vec{r}, t)} \Psi(\vec{r}, t) ; \quad \sigma \in \mathbb{R}$$

↑  
Lokalna transt.  
(na vsakem  $\vec{r}$  je lahko  $\sigma$  drugačen)

To damo v SE:

$$i\hbar \frac{\partial}{\partial t} \Psi' = \frac{1}{2m} \left( -i\hbar \nabla - \frac{e\vec{A}'}{\hbar} \right)^2 \Psi' + e\phi' \Psi'$$

$f_{Ax}$



## (Priprava / stranski račun)

$$(i \frac{\partial}{\partial x} + f) e^{i\sigma} \psi = - \left( \frac{\partial \sigma}{\partial x} \right) e^{i\sigma} \psi + e^{i\sigma} i \left( \frac{\partial \psi}{\partial x} \right) + f e^{i\sigma} \psi =$$

$$= e^{i\sigma} \left( i \frac{\partial}{\partial x} + \left( f - \frac{\partial \sigma}{\partial x} \right) \right) \psi$$

$$\left( i \frac{\partial}{\partial x} + f \right)^2 e^{i\sigma} \psi = \left( i \frac{\partial}{\partial x} + f \right) e^{i\sigma} \left( i \frac{\partial}{\partial x} + \left( f - \frac{\partial \sigma}{\partial x} \right) \right) \psi =$$

$$= e^{i\sigma} \left( i \frac{\partial}{\partial x} + \left( f - \frac{\partial \sigma}{\partial x} \right) \right)^2 \psi \quad e^{i\sigma} \neq 0$$

$$i\hbar \frac{\partial}{\partial t} \Psi = \frac{1}{2m} \sum_{\alpha} \left( -i\hbar \frac{\partial}{\partial x_{\alpha}} - eA'_{\alpha} + \hbar \frac{\partial \sigma}{\partial x_{\alpha}} \right)^2 \Psi + \left( e\phi' + \hbar \frac{\partial \sigma}{\partial t} \right) \Psi$$

x, y, z

$$i\hbar \frac{\partial}{\partial t} = \left[ \frac{(\vec{p} - e\vec{A})^2}{2m} + e\phi \right] i \quad \Lambda = \frac{\hbar}{e} \sigma$$

Torej če  $\Psi'$  po transformaciji  $\vec{A} \rightarrow \vec{A}'$  izrazi kot:

$$\underline{\underline{\Psi'(\vec{r}, t) = e^{i \frac{e}{\hbar} \Lambda(\vec{r}, t)} \Psi(\vec{r}, t)}}$$

$$\underline{\underline{g' = |\Psi'|^2 = |\Psi|^2 = g(\vec{r}, t)}}$$

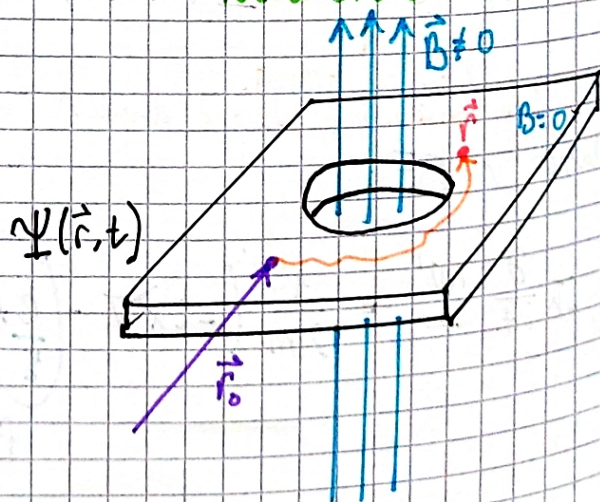
Neodvisno od umeritve

## Aharonov - Bohrov pojav

$$\vec{B} = \nabla \times \vec{A} = 0$$

$$\vec{A} = \nabla \Lambda$$

$$\Lambda(\vec{r}, t) = \Lambda(\vec{r}_0, t) - \int_{\vec{r}_0}^{\vec{r}} \vec{A}(\vec{r}') \cdot d\vec{r}'$$



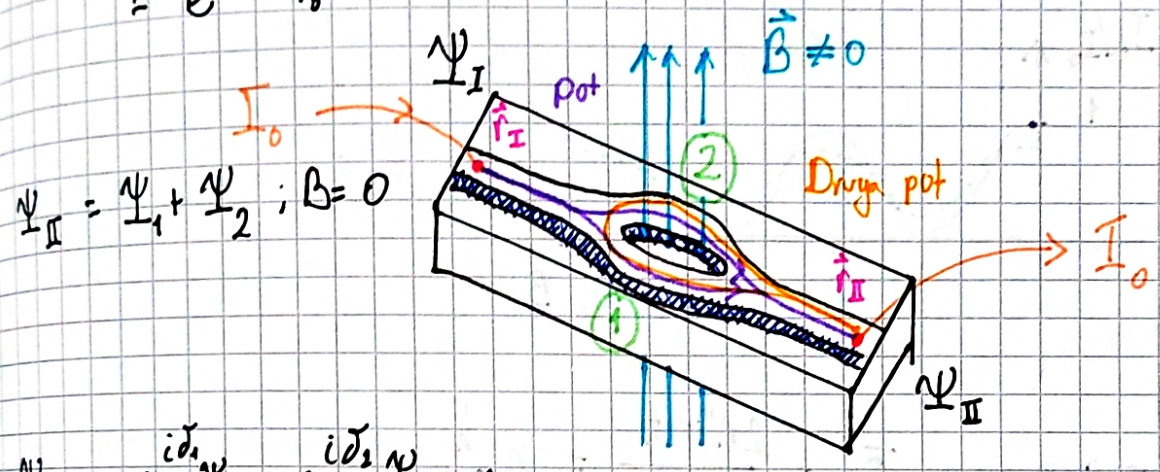


$$\Psi_A: i\hbar \frac{\partial \Psi_A}{\partial t} = \frac{(\hat{p} - e\vec{A})^2}{2m} \Psi_A + V\Psi_A \quad ; \quad \vec{B} = 0$$

$$\Psi_0: i\hbar \frac{\partial \Psi_0}{\partial t} = \frac{\hat{p}^2}{2m} \Psi_0 + V\Psi_0$$

$$\vec{A}' = \vec{A} + \nabla(-\Lambda) = 0$$

$$\Psi_A(\vec{r}, t) = e^{-i\frac{e}{\hbar}\Lambda(\vec{r}, t)} \Psi_0 = e^{i\frac{e}{\hbar} \int_{\vec{r}_0}^{\vec{r}} \vec{A}(\vec{r}') \cdot d\vec{r}'} \Psi_0(\vec{r}, t)$$



$$\Psi_{II} = \Psi_1 + \Psi_2 \quad ; \quad B = 0$$

$$\Psi_{IIA} = e^{i\delta_1} \Psi_1 + e^{i\delta_2} \Psi_2$$

$$\delta_1 = \frac{e}{\hbar} \int_{\vec{r}_I}^{\vec{r}_{II}} \vec{A}(\vec{r}') \cdot d\vec{r}'$$

2  
pot 1  
pot 2

$$\Psi_1 \approx \Psi_2$$

$$\Psi_{IIA} = e^{i\delta_1} \Psi_1 + e^{i\delta_2} \Psi_2 = e^{i\delta_2} (e^{i(\delta_1 - \delta_2)} \Psi_1 + \Psi_2) = e^{i\delta_2} (1 + e^{i(\delta_1 - \delta_2)}) \Psi_1$$

$$\delta_1 - \delta_2 = \frac{e}{\hbar} \oint_{\text{pot}} \vec{A}(\vec{r}') \cdot d\vec{r}' = \frac{e}{\hbar} \left( \int_{\text{pot 1}}^{\text{II}} \vec{A}(\vec{r}') \cdot d\vec{r}' - \int_{\text{pot 2}}^{\text{II}} \vec{A}(\vec{r}') \cdot d\vec{r}' \right) =$$

$$= \frac{e}{\hbar} \iint_S (\nabla \times \vec{A}) \cdot d\vec{S} = \frac{e}{\hbar} \iint_S \vec{B} \cdot d\vec{S} = \frac{e}{\hbar} \Phi_B$$

Magnetni pretok (ukljuko merimo)



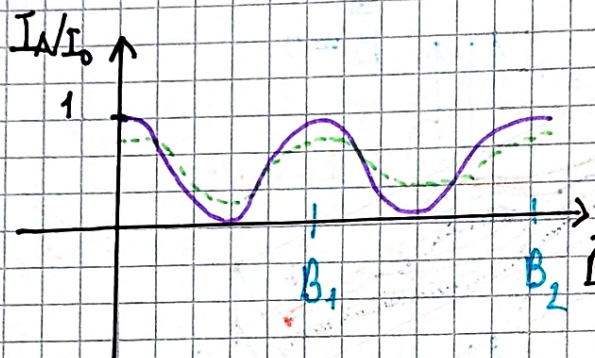
$$\frac{I_A}{I_0} = \frac{|\Psi_{IA}|^2}{|\Psi_{I0}|^2} = |1 + e^{i\frac{e}{\hbar}\Phi_B}|^2 \cdot \frac{1}{4} = \text{od tega ko ni polja } (1+1)^2$$

$$= \cos^2\left(\frac{e}{2\hbar}\Phi_B\right)$$

Torej je to:

$$I_A = I_0 \cos^2\left(\frac{e}{2\hbar}\Phi_B\right)$$

Aharonov-Bohmov pojav



Za maksimum:

$$\frac{e}{2\hbar}\Phi_B = \pi n ; \quad \Phi_B = \frac{2\pi\hbar}{e} = n \frac{h}{e}$$

Iz tega lahko naredijo sonde za merjenje magnetnega polja zelo natančno (SQUID)

## Spin

Pri pogledu o vrtilni količini smo videli:

$$\vec{L}: \quad L = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \quad [L_\alpha, L_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} L_\gamma$$

$\begin{matrix} \downarrow & \downarrow \\ \text{Nezvečno} & \text{m} \end{matrix}$

Pri spinih bomo pa polarizacijo pustili in bomo videli, kam prideemo.

$$[S_\alpha, S_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} S_\gamma$$

$$S = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$$

$$S_\pm = S_x \pm iS_y$$



$$|sm_s\rangle = |sm\rangle = \left| \frac{1}{2} m \right\rangle = |m\rangle = \begin{pmatrix} |\uparrow\rangle \frac{1}{2} \\ |\downarrow\rangle -\frac{1}{2} \end{pmatrix} \text{ @ Znak$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}; \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \text{ Spinor}$$

Analogno kot prej:

$$S_{\pm} |sm\rangle = \hbar \sqrt{(s+1)s - m(m \pm 1)} |sm \pm 1\rangle$$

$$S_z |sm\rangle = m\hbar |sm\rangle$$

$$\vec{S} = (S_x, S_y, S_z)$$

$$\vec{S}^2 |sm\rangle = s(s+1)\hbar^2 |sm\rangle$$

Odtod zdaj gledamo  $s = 1/2$

$$S_+ |\downarrow\rangle = \hbar |\uparrow\rangle$$

$$S_- |\uparrow\rangle = \hbar |\downarrow\rangle$$

(\*) kot prej

$$L_+ Y_l^l = 0$$

$$L_- Y_l^{-l} = 0$$

Poglejmo matrične elemente:

$$\langle \uparrow | S_+ | \uparrow \rangle = 0 = \langle \downarrow | S_+ | \downarrow \rangle$$

$$\langle \downarrow | S_+ | \uparrow \rangle = 0 \quad \langle \uparrow | S_+ | \downarrow \rangle = \hbar$$

(\*) = 0

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$(S_+)^{\dagger} = S_-$$

$$S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$l=1: L_x = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$$

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = S_x^{\dagger}$$

$$S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{!}$$

$$S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{!}$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_y = \frac{1}{2i}(S_+ - S_-) = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = S_y^{\dagger}$$

$$\begin{matrix} |\uparrow\rangle & |\downarrow\rangle \\ |\uparrow\rangle & \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \\ |\downarrow\rangle & \end{matrix}$$







$$\cdot \partial_x \partial_y b_z = i \mathbb{I}$$

$$\cdot \partial_x \partial_y = i \partial_z = -\partial_y \partial_x \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\cdot \partial_\alpha \partial_\beta = \delta_{\alpha\beta} \mathbb{I} + i \epsilon_{\alpha\beta\gamma} \partial_\gamma$$

$$\cdot [\partial_\alpha, \partial_\beta] = 2i \epsilon_{\alpha\beta\gamma} \partial_\gamma$$

$$\cdot \{\partial_\alpha, \partial_\beta\} = \partial_\alpha \partial_\beta + \partial_\beta \partial_\alpha = 2\delta_{\alpha\beta} \mathbb{I}$$

$$\cdot \vec{\partial} = (\partial_x, \partial_y, \partial_z)$$

$$\cdot \vec{a} = (a_x, a_y, a_z)$$

$$\vec{a} \cdot \vec{\partial} = \sum_\alpha a_\alpha \partial_\alpha$$

$$\cdot \underbrace{(\vec{a} \cdot \vec{\partial}) \cdot (\vec{b} \cdot \vec{\partial})}_{\text{green wavy}} = \sum_{\alpha\beta} a_\alpha \partial_\alpha b_\beta \partial_\beta = \underbrace{\vec{a} \cdot \vec{b} \mathbb{I} + i(\vec{a} \times \vec{b}) \cdot \vec{\partial}}_{\text{green wavy}}$$

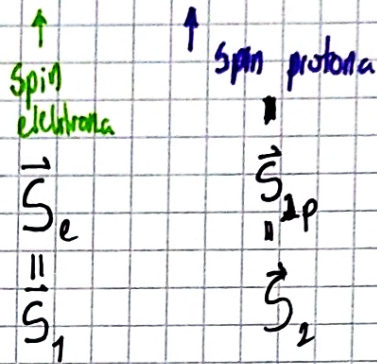
$$\vec{a} = \vec{b} = \vec{n} ; |\vec{n}| = 1$$

$$(\vec{n} \cdot \vec{\partial})(\vec{n} \cdot \vec{\partial}) = \mathbb{I}$$



# Sestevanje vrtilnih količin (cont.)

$$|\Psi\rangle = |\frac{1}{2} m_e\rangle |\frac{1}{2} m_p\rangle$$



$$\vec{S}_1 = \frac{\hbar}{2} \vec{\sigma}_1 = \frac{\hbar}{2} (\sigma_x, \sigma_y, \sigma_z)_1 \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_1$$

Vpeljemo še tenzorski produkt  $\otimes$ .

Baza za 2 dela

$$|\alpha_1, m_1\rangle \otimes |\alpha_2, m_2\rangle = |\Psi\rangle$$

$$\vec{S}_1 |\Psi\rangle = |\tilde{\Psi}\rangle$$

Hocemo da  $\uparrow$   
deluje le na prvi del

$$\vec{S}_1 \rightarrow \vec{S}_1 \otimes I_2$$

$\uparrow$  deluje na prvi vektor  
 $\uparrow$  nič ne naredi na drugem vektorju

Poseben primer:

$$\phi(x, y); \quad A = \frac{\partial}{\partial x} \quad B = \frac{\partial}{\partial y}$$

$$C = A + B$$

$$C\phi = \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y}$$

$$\phi(x, y) = \phi_1(x)\phi_2(y)$$

$$C\phi = \hbar \frac{\partial \phi_1}{\partial x} \phi_2 + \frac{\partial \phi_2}{\partial y} \phi_1$$

$$C = A \otimes I_y + I_x \otimes B$$

$$\phi = \phi_1(x) \otimes \phi_2(y)$$

V tem duhu je operator celotne vrtilne količine:

$$\vec{S} = \vec{S}_1 \otimes I_2 + I_1 \otimes \vec{S}_2$$

$$\because \alpha_1 = \frac{1}{2} = \alpha_2; \text{ baza}$$

$m \rightarrow \uparrow$  ali  $\downarrow$

$$|\uparrow\rangle \otimes |\uparrow\rangle$$

$$|\uparrow\rangle \otimes |\downarrow\rangle$$

$$|\downarrow\rangle \otimes |\uparrow\rangle$$

$$|\downarrow\rangle \otimes |\downarrow\rangle$$



Poglejmo bolj konkretni primer:

$$S_z = S_{1z} \otimes I_2 + I_1 \otimes S_{2z}$$

$$S_z |m_1\rangle \otimes |m_2\rangle = S_{1z} \otimes I_2 |m_1\rangle \otimes |m_2\rangle + I_1 \otimes S_{2z} |m_1\rangle \otimes |m_2\rangle =$$

delje  $m_1$                       delje  $m_2$

$$= m_1 |m_1\rangle \otimes |m_2\rangle + m_2 |m_1\rangle \otimes |m_2\rangle = (m_1 + m_2) |m_1\rangle \otimes |m_2\rangle$$

emiselni  $\otimes$

$m = m_1 + m_2$

$m = -1, 0, 1$

Poglejmo si komutator:

$$[S_\alpha, S_\beta] = [S_{1\alpha} \otimes I_2 + I_1 \otimes S_{2\alpha}, S_{1\beta} \otimes I_2 + I_1 \otimes S_{2\beta}] =$$

$$= [S_{1\alpha}, S_{1\beta}] \otimes I_2 + I_1 \otimes [S_{2\alpha}, S_{2\beta}] + 0 + 0 =$$

$[I_1, S_2]$   
isto drugi prostor

$$= i\hbar \epsilon_{\alpha\beta\gamma} S_{1\gamma} \otimes I_2 + I_1 \otimes i\hbar \epsilon_{\alpha\beta\gamma} S_{2\gamma}$$

$$\Rightarrow [S_\alpha, S_\beta] = i\hbar \epsilon_{\alpha\beta\gamma} S_\gamma$$

Spet standardna komutacijska zveza za VK. Kot pričakovano.

To pomeni, da lahko kot pri posameznih VK vpijemo:

$$S_\pm = S_x \pm iS_y = S_{1\pm} I_2 + I_1 \otimes S_{2\pm}$$



$$\therefore \vec{S}^2 |l m\rangle$$

Stanje dveh delcev

$$\vec{S}^2 |l m\rangle = \hbar^2 l(l+1) |l m\rangle$$

$$S_z |l m\rangle = \hbar m |l m\rangle$$

$\otimes m = m_1 + m_2 = \{-1, 0, 1\} \rightarrow l = 0$  ali  $1$

Zanimajo nas lastna stanja  $|l m\rangle \dots$

$$|l m\rangle = \sum_{m_1, m_2} C_{m_1, m_2} |m_1\rangle \otimes |m_2\rangle$$

navada  $\nabla$

$$m = m_1 + m_2 = \{-1, 0, 1\}$$

$$|m_1\rangle |m_2\rangle$$

$$l = \{0, 1\}$$

$$|m_1 m_2\rangle \Rightarrow |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$$

Nikoli ju oboje zamenjati

a)  $l = 1$

$$m=1 \quad S^2 |1 m\rangle = 1(1+1)\hbar^2 |1 m\rangle = 2\hbar^2 |1 m\rangle$$

$$S_z |1 1\rangle = \hbar |1 1\rangle = \hbar |\uparrow\uparrow\rangle \quad \text{reda bo } l=1$$

Torej:  $|2m\rangle = |1 1\rangle = |\uparrow\rangle \otimes |\uparrow\rangle = |\uparrow\uparrow\rangle$

$$m=0 \quad S_- |1 1\rangle = \sqrt{l(l+1) - m(m-1)} \hbar |1, 0\rangle$$

$$S_- |1 1\rangle = \sqrt{2} \hbar |1 0\rangle$$

Naredimo še isto operacijo na drug način

$$(S_{1-} \otimes I_2 + I_1 \otimes S_{2-}) |\uparrow\rangle \otimes |\uparrow\rangle = S_{1-} \otimes I_2 |\uparrow\uparrow\rangle + I_1 \otimes S_{2-} |\uparrow\uparrow\rangle = \hbar (|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)$$

Spin-flip

$$S_{1+} |\uparrow\rangle = \hbar |\uparrow\rangle$$

$$S_{1+} |\downarrow\rangle = 0$$

$$S_{1-} |\uparrow\rangle = 0$$

$$S_{1-} |\downarrow\rangle = \hbar |\downarrow\rangle$$



To dvoje enačimo:

$$\hbar(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = \sqrt{2}\hbar|10\rangle$$

$$|10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

~~...~~  
 $m = -1$

$$|1, -1\rangle = |2m\rangle = |\downarrow\downarrow\rangle$$

$$S_-|10\rangle = \dots \propto |1, -1\rangle$$

$Q = 1$ :

$$m = 1 \quad |\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$$

$$m = 0 \quad |10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

$$m = -1 \quad |\downarrow\downarrow\rangle = |\downarrow\downarrow\rangle$$

Tripletna stanja

$Q = 0$ :  $m = 0 \quad |00\rangle = c_1|\uparrow\downarrow\rangle + c_2|\downarrow\uparrow\rangle$

Mora veljati  $\langle 10|00\rangle = 0$

$$\Rightarrow |00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \text{Singletno stanje}$$

Primer: Heisenbergova spinovitev

Smo se navadili na tenzorske:

Klasiko:  $\uparrow \nearrow \quad H \propto \vec{p}_1 \cdot \vec{p}_2$

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

kvantno:  $H = J_0 \vec{S}_1 \cdot \vec{S}_2$

Iščemo znova  $H|\Psi\rangle = E|\Psi\rangle$

$$\vec{S} \cdot \vec{S} = (\vec{S}_1 + \vec{S}_2) \cdot (\vec{S}_1 + \vec{S}_2) = S_1^2 + S_2^2 + 2\vec{S}_1 \cdot \vec{S}_2$$

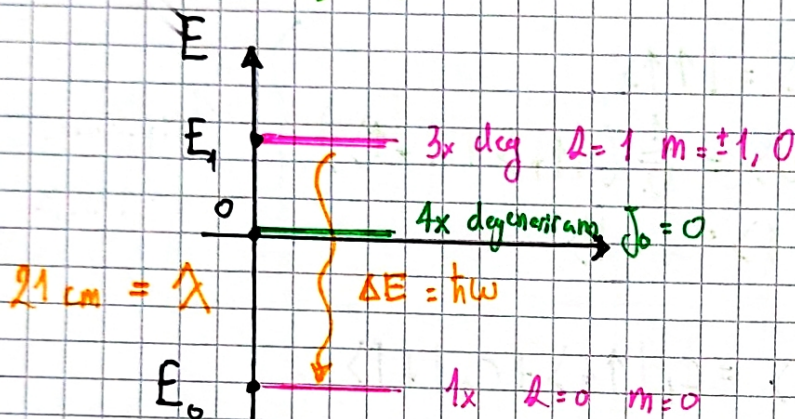
$$\frac{3}{4}\hbar^2 = \frac{1}{2}(\frac{1}{2}+1)\hbar^2$$

$$\Rightarrow H = \frac{J_0}{2} \left( S^2 - \frac{3}{4}\hbar^2 \right)$$



$$H|l m\rangle = \underbrace{\frac{J_0 \hbar^2}{2} (l(l+1) - \frac{3}{4})}_{E_l} |l m\rangle$$

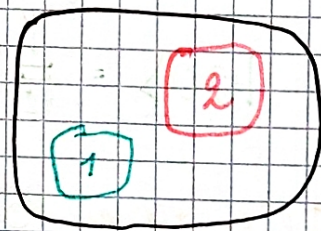
$$E_l = J_0 \hbar^2 \begin{cases} \frac{1}{4} & ; l=1 \\ -\frac{3}{4} & ; l=0 \end{cases}$$



### Clebsch-Gordanovi koeficienti

$$\vec{J}_1, J_{1z}$$

$$\vec{J}_2, J_{2z}$$



Kvantni sistem dveh strari/delcev

$$[J_{\alpha\alpha}, J_{\beta\beta}] = i\hbar \epsilon_{\alpha\beta\gamma} J_{\alpha\alpha} S_{\beta\gamma}$$

$$\vec{J} = \vec{J}_1 \otimes I_2 + I_1 \otimes \vec{J}_2 = \vec{J}_1 + \vec{J}_2$$

$$\vec{J}_1 = \vec{L}_{11}, \vec{S}_{11}, \vec{J}_1, \dots$$

baza:  $|j_1 m_1\rangle \otimes |j_2 m_2\rangle = |j_1 m_1 j_2 m_2\rangle$

št. bazis. rel.  $(2j_1+1) (2j_2+1)$

$\vec{J}_1 = \vec{L}_1, \vec{J}_2 = \vec{S}_2$   $2(2l+1) \rightarrow$  število je enako en delcu



$$|j, m\rangle = |j_1 j_2 j, m\rangle$$

Recimo  $l=1, m=0$  stanje vodila:  $|\frac{1}{2} \frac{1}{2} 1 0\rangle$

$$|j_1 j_2 j, m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 m_1\rangle |j_2 m_2\rangle \underbrace{\langle j_1 m_1, j_2 m_2 | j, m\rangle}_{C_{j_1 m_1 j_2 m_2}^{j m} \in \mathbb{C}}$$

Clebsch-gordanov koeficijent

$$C \neq 0: m = m_1 + m_2$$

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

a)  $\left. \begin{matrix} m_1 = \frac{1}{2} \\ m_2 = -\frac{1}{2} \end{matrix} \right\} m = \frac{1}{2}$

b)  $\left. \begin{matrix} m_1 = 0 \\ m_2 = \frac{1}{2} \end{matrix} \right\} m = \frac{1}{2}$

Primer uporabe tabel:

$$l=1 \quad \Psi = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 \\ Y_{1=1} \\ Y_{1=-1} \end{pmatrix} - \sqrt{\frac{1}{3}} \begin{pmatrix} Y_{1=0} \\ 0 \\ 0 \end{pmatrix}; \quad j = \frac{1}{2} \quad m = \frac{1}{2}$$

$$l = \frac{1}{2}$$

$$|j, m\rangle = ?$$

$$|j_1 j_2 j, m\rangle = |1 \frac{1}{2} \frac{1}{2} \frac{1}{2}\rangle \quad \begin{matrix} |+\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ |-\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{matrix}$$

$$\Rightarrow |1 \frac{1}{2} \frac{1}{2} \frac{1}{2}\rangle = \sqrt{\frac{2}{3}} |1 1\rangle | \frac{1}{2}, -\frac{1}{2}\rangle - \sqrt{\frac{1}{3}} |1 0\rangle | \frac{1}{2}, \frac{1}{2}\rangle$$

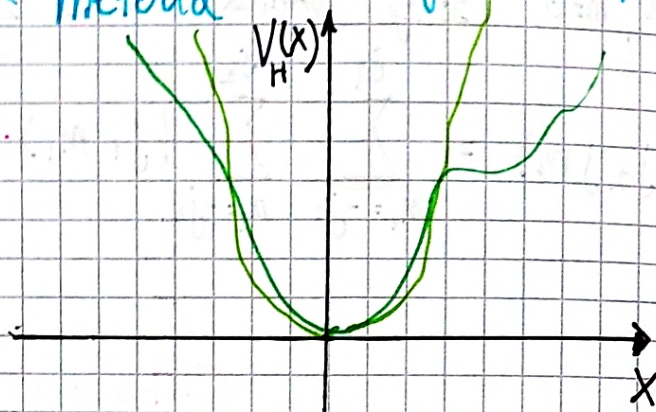
$\begin{matrix} l & s & j & m & & l & m_1 & l & m_2 \end{matrix}$



# Teorija motenj (perturbacij)

## 1. Rayleigh - Schrödingerjeva metoda (za nede degeneriran spekter)

$$H = \underbrace{\frac{p^2}{2m}}_{H_0} + \frac{1}{2} kx^2 + \underbrace{\alpha x^3}_{\text{popravek}} + \underbrace{\beta x^4}_{\text{popravek}} + \dots$$



$$H_{\text{op}} = H_0 + H_1$$

↑  
ničti približek

$$H_0 |n^0\rangle = E_n^{(0)} |n^0\rangle ; \langle m^0 | n^0 \rangle = \delta_{m,n}$$

nede degenerirana  
baza

Parametrizirajmo motnjo:

$$H_1 = \lambda V ; \hat{V} = V \quad \begin{array}{l} \lambda \text{ brezdimenzijski parameter} \\ \text{(lahko tudi huj zelo kompliciranega)} \end{array}$$

$$H |n\rangle = E_n |n\rangle$$

$$\begin{array}{l} \lambda \rightarrow 1 \\ H_1 \rightarrow \hat{V} \end{array}$$

Hočemo:

$$|n\rangle = |n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \dots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

$$\langle n^0 | n^0 \rangle \neq 0$$

$$\langle n^0 | n^0 \rangle = 1 + \lambda \underbrace{\langle n^0 | n^1 \rangle}_0 + \lambda^2 \underbrace{\langle n^0 | n^2 \rangle}_0 + \dots \quad \neq 1$$

Vsi popravki ortogonalni

Na koncu pa še renormiramo  $\langle n | n \rangle = 1$ .



$$(H_0 + \lambda V)(|n^0\rangle + \lambda |n^1\rangle + \dots) = (E_n^{(0)} + \lambda E_n^{(1)} + \dots)(|n^0\rangle + \lambda |n^1\rangle + \dots)$$

Pogledamo člen pr. istic potencak  $\lambda$ :

$$\lambda^0: H_0 |n^0\rangle = E_n^{(0)} |n^0\rangle \quad / \cdot \langle n^0|$$

$$\lambda^1: H_0 |n^1\rangle + V |n^0\rangle = E_n^{(0)} |n^1\rangle + E_n^{(1)} |n^0\rangle$$

$$\lambda^2: H_0 |n^2\rangle + V |n^1\rangle = E_n^{(0)} |n^2\rangle + E_n^{(1)} |n^1\rangle + E_n^{(2)} |n^0\rangle \quad / \langle n^0|$$

$$\Rightarrow \langle n^0 | H_0 |n^1\rangle + \langle n^0 | V |n^0\rangle = E_n^{(0)} \underbrace{\langle n^0 | n^1 \rangle}_0 + E_n^{(1)} \underbrace{\langle n^0 | n^0 \rangle}_1 =$$

$$\Rightarrow E_n^{(1)} = V_{nn}$$

$$I = \sum_m |m^0\rangle \langle m^0|$$

$$|n^1\rangle = I |n^1\rangle = \sum_{m \neq n} |m^0\rangle \underbrace{\langle m^0 | n^1 \rangle}_{\text{koeficienti}}$$

Tako razvib funkcijo damo nazaj in pomnožimo  $\langle m^0|$

$$\lambda^1: \langle m^0 | H_0 |n^1\rangle + \langle m^0 | V |n^0\rangle = \langle m^0 | E_n^{(0)} |n^1\rangle + \langle m^0 | E_n^{(1)} |n^0\rangle$$

o stanja med sabo ortogonalna

$$|n^1\rangle = \sum_{m \neq n} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} |m^0\rangle$$

To je popravek reda 1.!



$$E_n^{(2)} = \langle n^0 | V | n^1 \rangle$$

$$\Rightarrow E_n^{(2)} = \sum_{m \neq n} \frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$E_n^{(2)} = \langle n^0 | V | n^1 \rangle = \sum_{m \neq n} \underbrace{\langle n^0 | V | m^0 \rangle}_{V_{nm}} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} =$$

$$= \sum_{m \neq n} \frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}}$$

Torej je potencilna vrsta:

$$E_n = E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum_{m \neq n} \frac{|V_{nm}|^2}{E_n^{(0)} - E_m^{(0)}} + \mathcal{O}(\lambda^3); \quad \lambda \rightarrow 1$$

$$|n\rangle = |n^0\rangle + \lambda \sum_{m \neq n} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} |m^0\rangle + \mathcal{O}(\lambda^2)$$

Renormiranje:

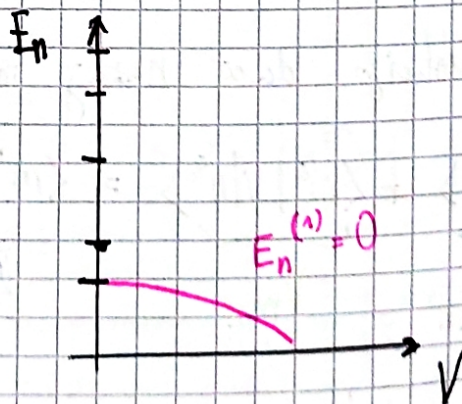
$$\langle n | n \rangle = (\langle n^0 | + \lambda \langle n^1 | + \mathcal{O}(\lambda^2)) (|n^0\rangle + \lambda |n^1\rangle + \mathcal{O}(\lambda^2))$$

$$= 1 + \mathcal{O}(\lambda^2) \quad \rightarrow \text{že normirano do drugega reda}$$

Naj bo  $E_n^{(0)}$  osnovno stanje  $n$ ;

$$E_n^{(0)} < E_m^{(0)} \quad \forall m$$

$$\Rightarrow E_n^{(2)} \leq 0$$



V drugem vedu perturbacije se vedno zniža energija osnovnega stanja.



## 2. Degeneriran speliter

$$H = H_0 + \lambda V$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

$$|n\rangle = C_1 |n_1^0\rangle + C_2 |n_2^0\rangle + \lambda |n^1\rangle + \dots$$

Pretpostavimo  $2 \times$  degeneracijo

$$H |n\rangle = E_n |n\rangle$$

Na vsaki strani spet visti

$$\lambda^0: H_0 |n_1^0\rangle = E_n^{(0)} |n_1^0\rangle$$

$$H_0 |n_2^0\rangle = E_n^{(0)} |n_2^0\rangle$$

$$+ E_n^{(1)} |n^1\rangle \} 0$$

$$\lambda^1: H_0 |n^1\rangle + C_1 V |n_1^0\rangle + C_2 V |n_2^0\rangle = E_n^{(1)} (C_1 |n_1^0\rangle + C_2 |n_2^0\rangle) \quad / \cdot \langle n_1^0 |$$

$$\underbrace{\langle n_1^0 |}_{0}$$

$$\langle n_1^0 |$$

$$\langle n_1^0 |$$

$$\underbrace{\langle n_1^0 |}_{1}$$

$$\underbrace{\langle n_1^0 |}_{1}$$

Torej:

$$E_n^{(1)} C_1 = V_{11} C_1 + V_{12} C_2$$

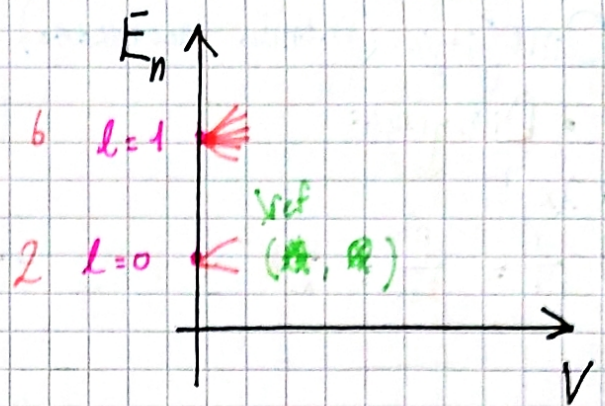
Če pa  $/ \cdot \langle n_2^0 |$  na začetku, dobimo:

$$E_n^{(1)} C_2 = V_{21} C_1 + V_{22} C_2$$

Dobimo problem lastnih vrednosti:

$$\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = E_n^{(1)} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$$

Dve rešitvi  
(\*) (\*)





## Omejitve (menda neobvezno)

• Divergence:

•  $\lambda x^m$

$$1) H = \frac{p^2}{2m} + \frac{k}{2} x^2 + \lambda x \quad \text{---> } (x-x_0)^2 + C$$

Premaknjeni LHO

$$2) E_n = E_n^0 + \sum_k c_k \lambda^k \quad ; \quad |\lambda| \leq \lambda_R$$

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2 + \lambda x^2$$

$$\frac{1}{2} k x^2 + \frac{1}{2} k \left( \frac{\lambda^2}{k} \right) x^2 = \frac{1}{2} k \left( 1 + 2 \frac{\lambda}{k} \right) x^2$$

$$k = m\omega^2$$

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 \left( 1 + 2 \frac{\lambda}{k} \right) x^2$$

$$E_n^{(0)} = \hbar\omega \left( n + \frac{1}{2} \right)$$

$$E_n = \hbar\omega \sqrt{1 + 2 \frac{\lambda}{k}} \left( n + \frac{1}{2} \right)$$

$$3) H = \frac{p^2}{2m} + \frac{1}{2} k x^2 + \lambda x^4 \Rightarrow \text{Asimptotski razvoj}$$

• fazni prehodi

$$1) \text{ Superprevodnost } \rightsquigarrow T_c \propto e^{-\frac{C}{\lambda}}$$

Se ne da razviti za male  $\lambda$

Torej potenčna vrsta nima smisla in ne gre.



# Brillouin Wignerjeva perturbacija (zanimivost/neobvezno)

$$H = H_0 + \lambda V$$

$$E_n = E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum_m \frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}} + \dots +$$

$$+ \lambda^j \sum_{\substack{m_1 \\ m_2 \\ \vdots \\ m_{j-1}}} \frac{V_{m_1 n} V_{m_1 m_2} V_{m_2 m_3} \dots V_{m_{j-1} n}}{(E_n^{(0)} - E_{m_1}^{(0)}) (E_n^{(0)} - E_{m_2}^{(0)}) \dots (E_n^{(0)} - E_{m_{j-1}}^{(0)})} \equiv T_{ni}^{(j)}(0)$$

Velja za degeneriran in nedegeneriran primer.

## Od časa odvisna motnja

$$H(t) = H_0 + \lambda \hat{V}(t)$$

Neodvisen od t

$\rightarrow -\vec{j} \cdot \vec{B}(t)$  recimo

$H_0 |n\rangle = E_n |n\rangle$ ;  $\{|n\rangle\}$  baza;  $\langle m|n\rangle = \delta_{mn}$

$$t=0: |\Psi(0)\rangle = \sum_n c_n(0) |n\rangle$$

$$t>0: |\Psi(t)\rangle = \sum_n c_n(t) e^{-i \frac{E_n t}{\hbar}} |n\rangle$$

To je naš nastavek za:

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = H(t) |\Psi(t)\rangle$$

$$i\hbar \sum_n \left( \frac{\partial c_n(t)}{\partial t} e^{-i \frac{E_n t}{\hbar}} - i \frac{E_n}{\hbar} c_n(t) e^{-i \frac{E_n t}{\hbar}} \right) |n\rangle = \sum_n (E_n + \lambda V(t)) e^{-i \frac{E_n t}{\hbar}} c_n(t) |n\rangle$$

Celo enačbo množimo z  $\langle m|$



$$i\hbar \frac{\partial c_m(t)}{\partial t} e^{-i \frac{E_m}{\hbar} t} = \lambda \sum_n \langle m | V(t) | n \rangle e^{-i \frac{E_n}{\hbar} t} c_n(t)$$

$$i\hbar \frac{\partial c_m(t)}{\partial t} = \lambda \sum_n \underbrace{\langle m | V(t) | n \rangle}_{V_{mn}(t)} e^{-i \frac{E_n - E_m}{\hbar} t} c_n(t)$$

$$\Rightarrow i\hbar \frac{\partial c_m(t)}{\partial t} = \lambda \sum_n V_{mn}(t) c_n(t) \quad \lambda = 1$$

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \\ \vdots \end{pmatrix} = \begin{pmatrix} V_{11}(t) & V_{12}(t) & \dots \\ \vdots & \vdots & \ddots \\ \dots & \dots & V_{mn}(t) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_m \\ \vdots \end{pmatrix}$$

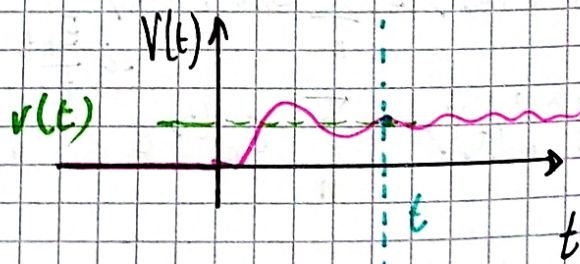
$$i\hbar \dot{\vec{c}} = \underline{V} \vec{c}$$

To je tačno!  $\forall i, c_i^1$

Temu se zove Diracova slika.

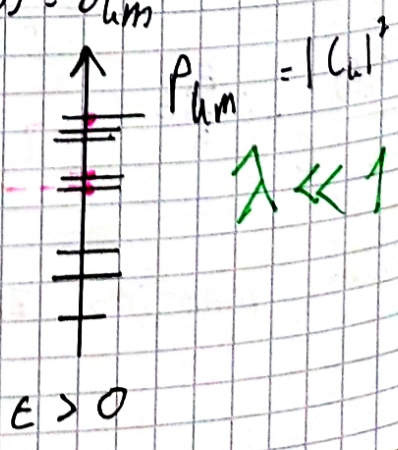
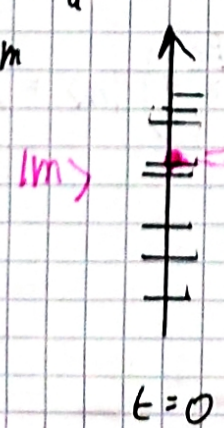
a) Šibler motnja

$$V(t) = \begin{cases} 0; & t \leq 0 \\ V(t); & t > 0 \end{cases}$$



$$|\Psi(0)\rangle = |m\rangle = \sum_u c_u(0) |u\rangle; \quad H_0, E_m$$

$$c_u(0) = \delta_{um}$$





$$|\psi(0)\rangle = |m\rangle = \sum_n 1 \cdot c_n(0) |n\rangle$$

$$c_n(0) = \delta_{nm}$$

$$|\psi(t)\rangle = \sum_n c_n(t) |n\rangle$$

$\Downarrow$

$$i\hbar \frac{\partial c_n}{\partial t} = \sum_m V_{nm} c_m(t) = \lambda V_{lm}(t)$$

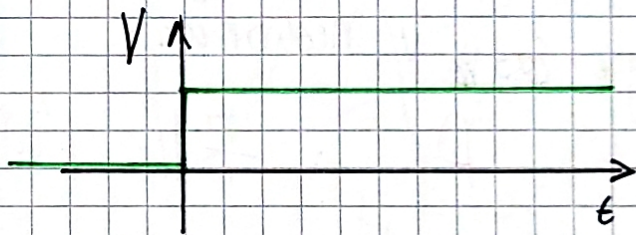
Rezultat:

$$c_l(t) = \frac{\lambda}{i\hbar} \int_0^t V_{lm}(t') dt'; \quad \text{za } l \neq m$$

$$c_m \approx 1; \quad \text{če } |c_l|^2 \ll 1.$$

Fermijevovo zlato pravilo

$$V(t) = \begin{cases} 0 & ; t \leq 0 \\ V & ; t > 0 \end{cases}$$



Tohrat vzamimo  $\langle m|V|n\rangle = V_{mn}$

$$c_l(t) = \frac{1}{i\hbar} \int_0^t V_{ml} e^{-i \frac{E_n - E_m}{\hbar} t'} dt' =$$

$$l \neq m$$

$$l = m \Rightarrow |c_m|^2 \approx 1$$

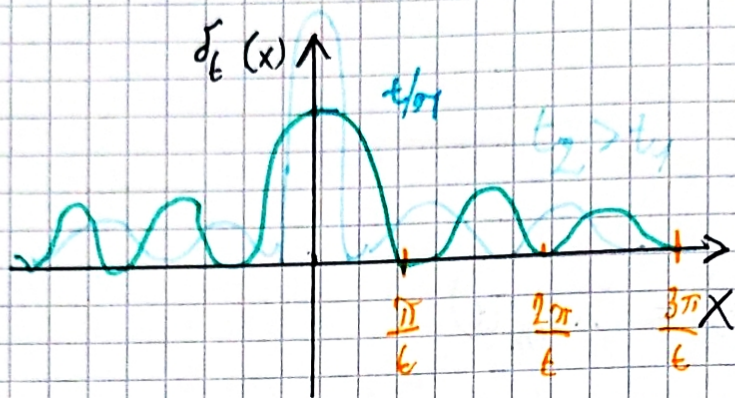
$$= \frac{V_{lm}}{i\hbar} \frac{e^{-i\omega_{lm}t} - 1}{-i\omega_{lm}}$$

$$X = \frac{1}{2} \frac{E_n - E_m}{\hbar} = \frac{1}{2} \omega_{lm}$$

$$\Rightarrow P_{lm} = \frac{|V_{lm}|^2}{\hbar^2} \frac{\sin^2\left(\frac{1}{2} \omega_{lm} t\right)}{(\omega_{lm})^2}$$



$$\delta_\epsilon(x) = \frac{1}{\pi} \frac{\sin^2 xt}{x^2 \epsilon} \quad ; \quad \int \delta_\epsilon(x) dx = 1$$



$\delta_\epsilon(x) \xrightarrow{\epsilon \rightarrow \infty} \delta(x)$  To je kot neka parametrizacija delte.

Velja:

$$P_{lum} = \frac{2\pi}{h} |V_{lum}|^2 \delta_x(E_\epsilon - E_m) \epsilon$$

$$\delta(ax) = \frac{1}{|a|} \delta(x)$$

Če negre ~~čas~~ v neskončen:

$$P_{lum} = \frac{2\pi}{h} |V_{lum}|^2 \delta_0(E_\epsilon - E_m) \epsilon$$

Približki:

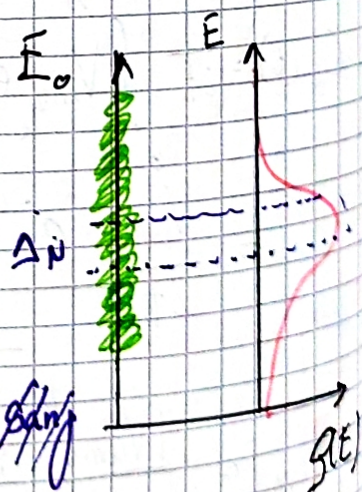
$$P_{lum} \ll 1$$

[Primer: gostota vezanih stanj]

$$g(E) = \frac{\Delta N}{\Delta E} \rightarrow \frac{dN}{dE}$$

$$P_{kumulj} : \sum_{u=m} P_{uonc} \rightarrow \int P_m(E) g(E_m) dE$$

gostota stanj



$$\Rightarrow P = \frac{2\pi}{h} [V_{lum}]^2 g(E_m) \epsilon \propto t$$



$$\frac{dP}{dt} = W = \frac{2\pi}{h} \dots$$

$$\frac{dP}{dt} = W = \frac{2\pi}{h} |V_{nm}|^2 \rho(E_n)$$

Fermijevo  
Zlato pravilo

[Primer:] Radiativnost

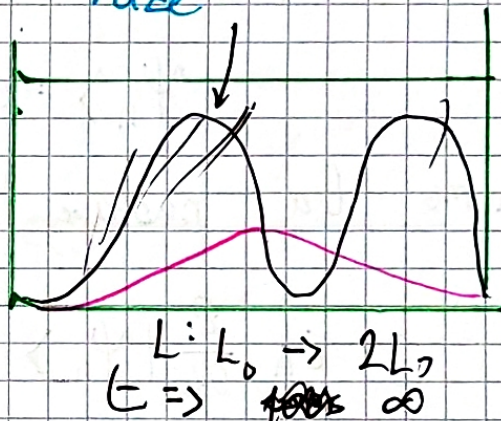
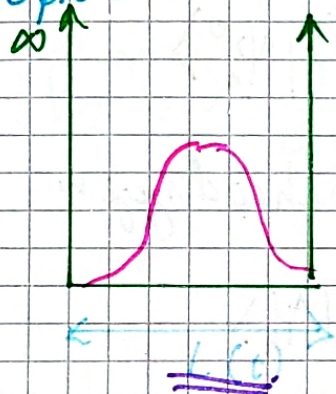
$$t=0: |\Psi(t)\rangle$$

Tolg za en prehodk:  $-dN = Npd = Nv dt$

Ni odvisnosti od časa / denarja:

Adiabatne ~~up~~ sprememba in kvantna faze Narobe

$H(t)$

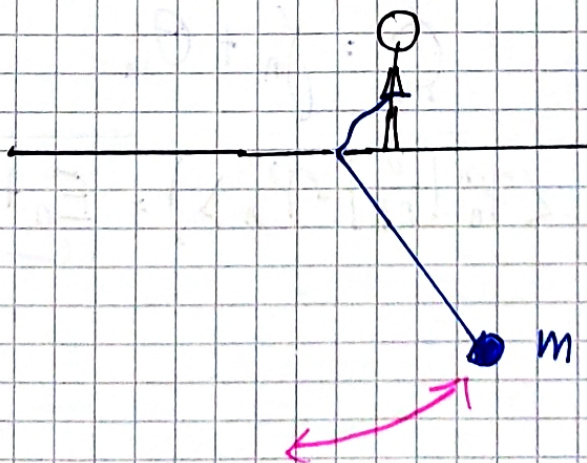


Zanima nas rešitev problema

$$\frac{dL}{dt} \ll \left( \frac{\Delta}{\hbar} \right) L; \Delta = \bar{E}_n - \bar{E}_m$$

$$\frac{dL}{dt} \ll \left( \frac{\Delta}{\hbar} \right) L; \Delta = \bar{E}_n - \bar{E}_m$$

Klasično je to lot:





$$H(\vec{Q}(t)) ; \vec{Q} = (L, V_0, \beta, \dots) = \vec{Q}(t)$$

$$\vec{Q} = (q_1, \dots, q_n)$$

$$t: H(\vec{Q}) |\Psi_n(\vec{Q})\rangle = E_n(\vec{Q}) |\Psi_n(\vec{Q})\rangle$$

$$\Psi_n^0(\vec{r}, t) = \langle \vec{r} | \Psi(\vec{Q}(t)) \rangle$$

Vstavimo v enačbo:

$$i\hbar \frac{\partial}{\partial t} |\Psi_n^0(\vec{r}, t)\rangle \neq H(\vec{Q}(t)) |\Psi_n^0\rangle$$

Adiabatski režim

Kvantna faza

$$|\Psi_n\rangle = e^{i\phi_n(t)} |\Psi_n^0\rangle$$

Nastavimo ta nastavek v Schrödingerovo enačbo:

$$i\hbar \frac{\partial}{\partial t} |\Psi_n\rangle = H |\Psi_n\rangle$$

$$i\hbar \left( i \frac{d\phi_n}{dt} e^{i\phi_n} |\Psi_n^0\rangle + e^{i\phi_n} |\Psi_n^0\rangle \right) = H e^{i\phi_n} |\Psi_n^0\rangle e^{i\phi_n} |\Psi_n^0\rangle$$

$$= e^{i\phi_n} E_n |\Psi_n^0\rangle$$

$$i\hbar \left( i \frac{d\phi_n}{dt} \langle \Psi_n^0 | \Psi_n^0 \rangle + \langle \Psi_n^0 | \frac{\partial}{\partial t} | \Psi_n^0 \rangle \right) =$$

$$= E_n \langle \Psi_n^0 | \Psi_n^0 \rangle$$

$$\phi_n = \gamma_n + \theta_n$$

$$i\hbar \left( i \frac{d\gamma_n}{dt} + \langle \Psi_n^0 | \frac{\partial}{\partial t} | \Psi_n^0 \rangle \right) = E_n + \hbar \frac{d\theta_n}{dt} = 0$$



$$\Rightarrow \frac{d\theta_n}{dt} = - \frac{E_n(\vec{Q}(t))}{\hbar}; \quad \theta_n = - \frac{1}{\hbar} \int_0^t E_n(t') dt'$$

$$\frac{dy_m}{dt} = c \langle \psi_n^0 | \frac{\partial}{\partial t} | \psi_n^0 \rangle$$

$$\frac{\partial}{\partial t} \psi_m = \sum_i \frac{\partial \psi_n^0}{\partial q_i} \dot{q}_i = (\vec{\nabla}_{\vec{Q}} \psi_n^0) \cdot \dot{\vec{Q}}$$

$$y = \int_0^t i \langle \psi_n^0 | \vec{\nabla}_{\vec{Q}} \psi_n^0 \rangle \cdot \dot{\vec{Q}} dt$$

$$y(t) = y_n \cdot \int_0^t i \langle \psi_n^0 | \vec{\nabla}_{\vec{Q}} \psi_n^0 \rangle \cdot \dot{\vec{Q}} dt = i \int_{\vec{Q}(0)}^{\vec{Q}(t)} \langle \psi_n^0 | \vec{\nabla}_{\vec{Q}} \psi_n^0 \rangle \cdot d\vec{Q}$$

Berryjeva faza:

$$y_m = i \oint \langle \psi_n^0 | \vec{\nabla}_{\vec{Q}} \psi_n^0 \rangle \cdot d\vec{Q}$$