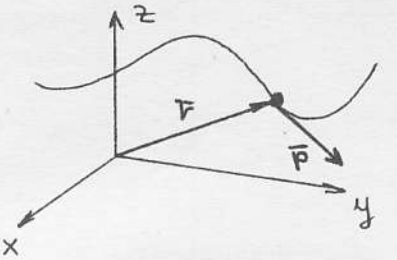
52

1.3. A perdület és a mágneses momentum

1.3.1. A pályaperdület

Klasszikus mechanika:

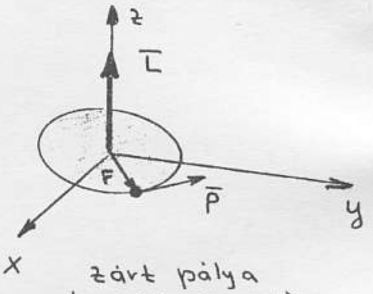


$$\boxed{\bar{L} = \bar{r} \times \bar{p}}$$

$L_x = \dots$

$L_y = \dots$

$L_z = x p_y - y p_x$



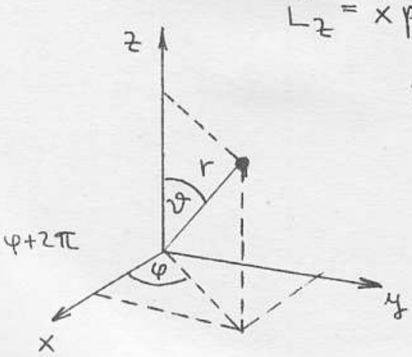
zárt pálya (kötött állapot)

Kvantummechanika:

(II. Axióma) $\hat{L}_x = \dots$

$\hat{L}_y = \dots$

$$\hat{L}_z = \hat{x}\hat{p}_y - y\hat{p}_x = \frac{\hbar}{j}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \longrightarrow \boxed{\hat{L}_z = \frac{\hbar}{j}\frac{\partial}{\partial \varphi}}$$



Bizonyítás:

$x = r \cdot \sin\vartheta \cdot \cos\varphi$

$y = r \cdot \sin\vartheta \cdot \sin\varphi$

$z = r \cdot \cos\vartheta$

$$\Phi(x,y,z) = \Phi(x(\varphi), y(\varphi)) = \Phi(\varphi)$$

$$\frac{\partial \Phi}{\partial \varphi} = \frac{\partial \Phi}{\partial x}\underbrace{\frac{\partial x}{\partial \varphi}}_{-y} + \frac{\partial \Phi}{\partial y}\underbrace{\frac{\partial y}{\partial \varphi}}_{x} =$$

(III. Axióma) $\hat{L}_z \Phi = L_z \Phi$

$$\frac{\hbar}{j}\frac{\partial}{\partial \varphi}\Phi = L_z \Phi \longrightarrow \Phi = A \cdot e^{j\frac{L_z}{\hbar}\varphi}$$ (matematikai megoldás)

(I. Axióma) $\Phi \in \mathcal{H} \longrightarrow$ regularitás: folytonos ✓ négyzetesen integrálható egyértékű

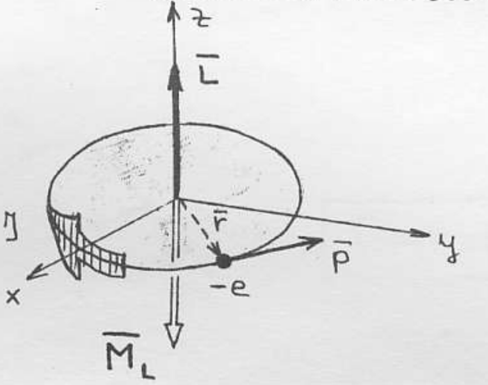
$$\langle \Phi | \Phi \rangle = |A|^2 2\pi = 1 \longrightarrow A = \frac{1}{\sqrt{2\pi}}$$

$$\Phi(\varphi + 2\pi) = \Phi(\varphi) \longrightarrow e^{j\frac{L_z}{\hbar}\varphi} \cdot \underbrace{e^{j\frac{L_z}{\hbar}2\pi}}_{1} = e^{j\frac{L_z}{\hbar}\varphi}$$

$\boxed{L_z = \hbar m_e}$ ($m_e = 0 \pm 1 \pm 2 \pm \dots$) (MÁGNESES kvantumszám) $\longleftarrow$ $\frac{L_z}{\hbar} \equiv m_e = 0 \pm 1 \pm 2 \pm 3 \pm \dots$

(53) 1.3.2. A (zárt) pályamozgás mágneses momentuma

Klasszikus mechanika:



$\bar{L}\,(0,0,L_z)$

$\bar{M}_L\,(0,0,M_z)$

$L_z = r \cdot p = r \cdot m \cdot v$

$M_z = J \cdot r^2 \pi$

$$J = \frac{dQ}{dt} = -\frac{e}{T} = -\frac{e}{\frac{2\pi r}{v}} = -\frac{ev}{2\pi r}$$

$$M_z = -\frac{ev}{2\pi r} \cdot r^2 \pi = -\frac{evr}{2} = -\frac{e}{2m} m \cdot v \cdot r = -\frac{e}{2m} L_z$$

$$\boxed{M_z = -\frac{e}{2m} L_z} \longrightarrow \boxed{\bar{M}_L = -\frac{e}{2m} \bar{L}}$$

Kvantummechanika:

(II. Axióma) $\hat{M}_x, \hat{M}_y, \hat{M}_z \longrightarrow \hat{M}_z = -\frac{e}{2m} \hat{L}_z$

(III. Axióma) $\hat{M}_z \Phi = M_z \Phi$

$$-\frac{e}{2m} \underbrace{\hat{L}_z \Phi}_{L_z \Phi} = M_z \Phi$$

$$M_z = -\frac{e}{2m} L_z = -\underbrace{\frac{e\hbar}{2m}}_{\equiv \mu_B} m_e$$

(BOHR magneton: a mágneses dipólmomentum kvantuma)

$$\boxed{M_z = -\mu_B \cdot m_e}$$

$(m_e = 0 \pm 1 \pm 2 \pm 3 \pm \ldots)$

$$\boxed{\Phi = \frac{1}{\sqrt{2\pi}} e^{j m_e \varphi}}$$

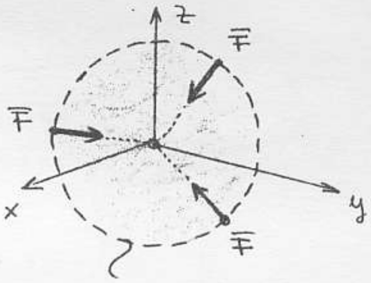
$\mu_B = 9{,}27 \cdot 10^{-24}\ \mathrm{Am}^2$

(54)

1.3.3. Mozgás centrális erőtérben

1.3.3.1. A pályaperdület meghatározása

Klasszikus mechanika:



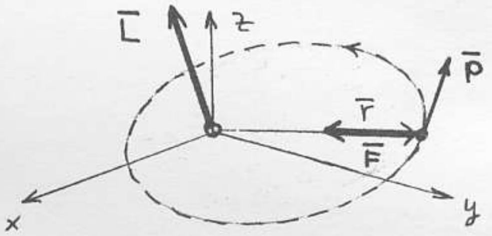
$V(\overline{F})$ = állandó

erő:

$$\overline{F}(\overline{r}) = F(r)\frac{\overline{r}}{r} \longrightarrow V(\overline{r}) = V(r)$$

$\downarrow$ pl.:

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



$$\overline{L} = \overline{r}\times\overline{p} \qquad \Big|\frac{d}{dt}$$

$$\frac{d\overline{L}}{dt} = \underbrace{\dot{\overline{r}}\times\overline{p}}_{\emptyset} + \overline{r}\times\dot{\overline{p}} = \underbrace{\overline{r}\times\overline{F}}_{\text{forgatónyomaték}}$$

Centrális erőtérben:

$$\dot{\overline{L}} = \overline{r}\times\overline{F} = \frac{F}{r}\underbrace{\overline{r}\times\overline{r}}_{\emptyset} \longrightarrow \boxed{\overline{L} = \text{áll}}$$

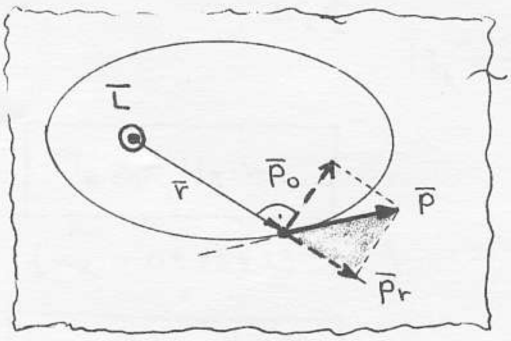
Konzervatív rendszerben $\boxed{E = \text{áll}}$

$$\text{Mivel } \overline{L} = \text{állandó} \longrightarrow \overline{r}\times\overline{p} = m\,\overline{r}\times\dot{\overline{r}} = \underbrace{m\cdot\overline{r}\times\frac{d\overline{r}}{dt}}_{\overline{r}\times d\overline{r}} = \text{állandó}$$

$\overline{r}\times d\overline{r}$ (iránya állandó)

$\downarrow$

SÍKMOZGÁS



a pálya síkja

$$\overline{p} = \overline{p}_0 + \overline{p}_r$$

$$\overline{L} = \overline{r}\times\overline{p} = \overline{r}\times\overline{p}_0 + \underbrace{\overline{r}\times\overline{p}_r}_{\emptyset}$$

$$\underline{L = r\cdot p_0}$$

$$H = \frac{p^2}{2m} + V(r) = \frac{p_r^2 + p_0^2}{2m} + V(r) = \frac{p_r^2}{2m} + \frac{p_0^2}{2m} + V(r) =$$

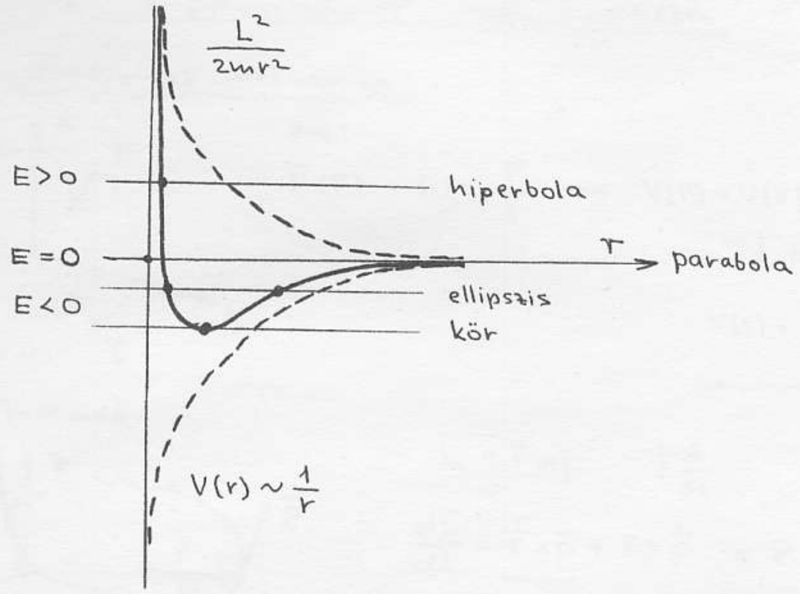
$$H = \frac{p_r^2}{2m} + \underbrace{\frac{L^2}{2mr^2} + V(r)}_{\equiv V_{eff}(r)} = E$$

$(L^2 = \text{állandó})$

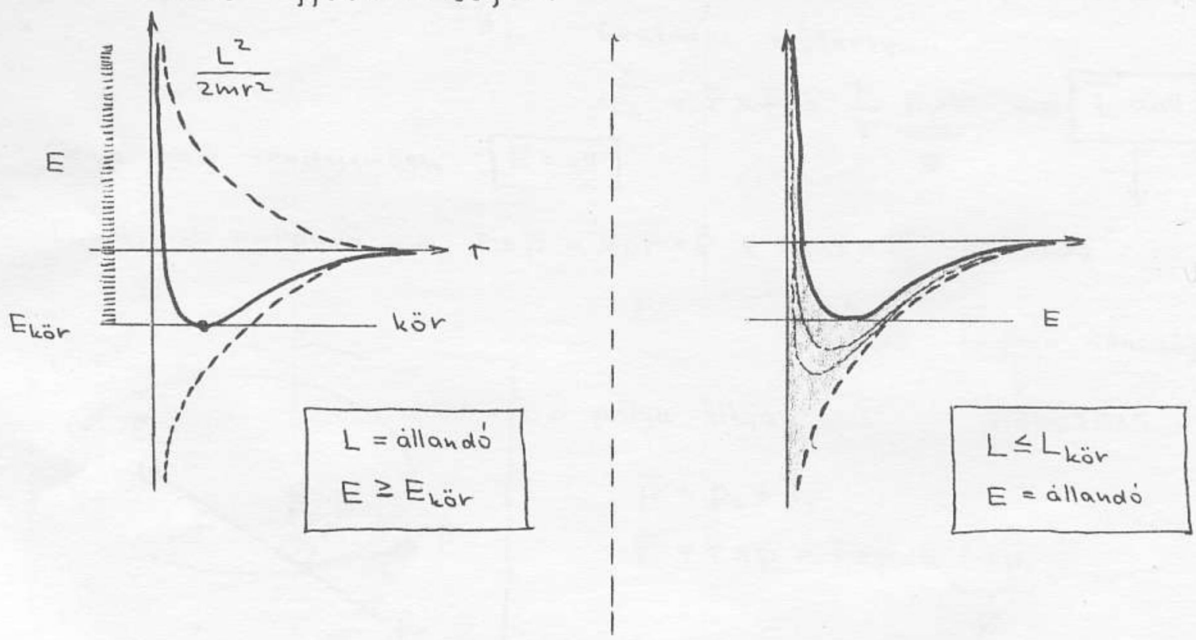
$$\boxed{\begin{aligned} H &= \frac{p_r^2}{2m} + V_{eff}(r) \\ V_{eff}(r) &= \frac{L^2}{2mr^2} + V(r) \end{aligned}}$$

(centrifugális potenciál)

55 Centrális erőtérben mozgó részecske pályájának jellemzése



Fontos egyenlőtlenségek:



(56) Kvantummechanika:

Klasszikus mechanika Hamilton függvény	Kvantummechanika Hamilton operátor

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(x,y,z) \longrightarrow \hat{H} = -\frac{\hbar^2}{2m}\Delta_{x,y,z} + V(x,y,z)$$

$\downarrow$ (Descartes) (polár)

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta_{r,\vartheta,\varphi} + V(r)$$

$$H = \frac{1}{2m}p_r^2 + \frac{1}{2mr^2}L^2 + V(r) \longrightarrow \hat{H} = \frac{1}{2m}\hat{p}_r^2 + \frac{1}{2mr^2}\hat{L}^2 + V(r)$$

Matematika:

$$\Delta_{r,\vartheta,\varphi} \equiv \Delta_r + \frac{1}{r^2}\Delta_{\vartheta,\varphi}$$

$$\Delta_r \equiv \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$$

$$\Delta_{\vartheta,\varphi} \equiv \underbrace{\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)}_{\equiv \Delta_\vartheta} + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$$

Tehát a $\hat{H}$ operátor polárkoordinátákkal felírva:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta_r - \frac{\hbar^2}{2mr^2}\Delta_{\vartheta,\varphi} + V(r)$$

$$\hat{H} = \frac{1}{2m}\hat{p}_r^2 + \frac{1}{2mr^2}\hat{L}^2 + V(r)$$

$$\hat{p}_r^2 = -\hbar^2\Delta_r$$

$$\boxed{\hat{L}^2 = -\hbar^2\Delta_{\vartheta,\varphi}} \longrightarrow \hat{L}^2 = -\hbar^2\Delta_\vartheta + \frac{1}{\sin^2\vartheta}\hat{L}_z^2$$

csererelációk:

$$\left.\begin{array}{l}[\hat{H},\hat{L}^2] = 0 \\ [\hat{L}^2,\hat{L}_z] = 0 \\ [\hat{H},\hat{L}_z] = 0\end{array}\right\} \longrightarrow \left.\begin{array}{l}\hat{H}\Psi = E\Psi \\ \hat{L}^2 Y = L^2 Y \\ \hat{L}_z\Phi = L_z\Phi\end{array}\right\} \quad (1.2.2)$$

$$\Psi(r,\vartheta,\varphi) = R(r)\,Y(\vartheta,\varphi) = R(r)\underbrace{\Theta(\vartheta)\,\Phi(\varphi)}_{\equiv Y(\vartheta,\varphi)}$$

57 A perdület sajátérték egyenlet megoldása:

$$\left.\begin{aligned} \hat{L}^2 Y &= L^2 Y \\ \hat{L}_z \Phi &= L_z \Phi \end{aligned}\right\} \quad Y(\vartheta,\varphi) = \Theta(\vartheta)\cdot\Phi(\varphi)$$

$$\left(-\hbar^2 \Delta_\vartheta + \frac{1}{\sin^2\vartheta}\hat{L}_z^2\right)\Theta\Phi = L^2\Theta\Phi$$

$$-\hbar^2 \Phi \Delta_\vartheta \Theta + \frac{\Theta}{\sin^2\vartheta}\underbrace{\hat{L}_z^2 \Phi}_{L_z^2\Phi} = L^2 \Theta \Phi \qquad \Big| \cdot \frac{1}{\Phi}$$

$$-\hbar^2 \Delta_\vartheta \Theta + \frac{L_z^2}{\sin^2\vartheta}\Theta = L^2 \Theta$$

$$\Delta_\vartheta \Theta + \Big(\underbrace{\frac{L^2}{\hbar^2}}_{\equiv A \text{ (jelölés)}} - \underbrace{\frac{L_z^2}{\hbar^2}}_{m_\ell^2}\frac{1}{\sin^2\vartheta}\Big)\Theta = 0 \quad \leftarrow \left\{ \begin{array}{l} \text{Ismeretes:} \\ L_z = \hbar m_\ell \\ m_\ell = 0 \pm 1 \pm 2 \pm \ldots \end{array}\right.$$

$$\boxed{\Delta_\vartheta \Theta + \left(A - \frac{m_\ell^2}{\sin^2\vartheta}\right)\Theta = 0}$$

megoldása polinom módszerrel

$$\rightarrow \left\{ \begin{array}{lll} \Theta(\vartheta) = P_\ell^{|m_\ell|}(\cos\vartheta) & & \text{(LEGENDRE)} \\ A = \ell(\ell+1) & \ell = 0,1,2,3,\ldots & \text{(neve: mellék kvantum szám)} \\ m_\ell = 0 \pm 1 \pm 2 \pm \ldots \pm \ell & & \end{array}\right.$$

Kapjuk tehát:

$$\boxed{\begin{array}{ll} Y(\vartheta,\varphi) = P_\ell^{|m_\ell|}(\cos\vartheta)\cdot e^{j m_\ell \varphi} & \\ L^2 = \hbar^2 \ell(\ell+1) & \ell = 0,1,2,3,\ldots \\ L_z = \hbar m_\ell & m_\ell = 0, \pm 1, \pm 2, \ldots \pm \ell \end{array}}$$

→ neve: GÖMBFÜGGVÉNY

A perdület komponensek közötti csererelációk:

$$\boxed{\begin{aligned} [\hat{L}_y, \hat{L}_z] &= -\frac{\hbar}{j}\hat{L}_x \\ [\hat{L}_z, \hat{L}_x] &= -\frac{\hbar}{j}\hat{L}_y \\ [\hat{L}_x, \hat{L}_y] &= -\frac{\hbar}{j}\hat{L}_z \end{aligned}}$$

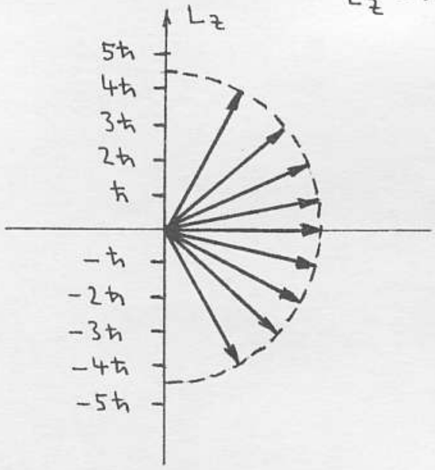
MÉRÉS (határozatlansági relációk)

58

A pályaperdület kvantálásának szemléltetése:

$$L = \hbar\sqrt{\ell(\ell+1)}$$

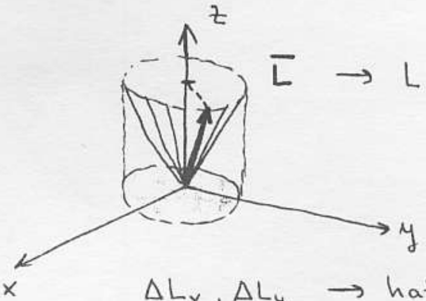
$$L_z = \hbar\, m_\ell \qquad (m_\ell = 0 \pm 1 \pm 2 \pm \ldots \pm \ell)$$



pl: $\ell = 4$

$L = \hbar\sqrt{4\cdot 5}$

$m_\ell = 0 \pm 1 \pm 2 \pm 3 \pm 4$



$\overline{L} \longrightarrow L_{z\,max} = \hbar\cdot\ell$

$\Delta L_x,\ \Delta L_y \longrightarrow$ határozatlansági relációból.

A pályamozgásból származó mágneses momentum:

$$\overline{M}_L = -\frac{e}{2m}\overline{L}$$

$$\hat{M}_L^2 = \left(\frac{e}{2m}\right)^2 \hat{L}^2 \longrightarrow \boxed{M_L = \mu_B\sqrt{\ell(\ell+1)}}$$

$$\hat{M}_z = -\frac{e}{2m}\hat{L}_z \longrightarrow \boxed{M_z = \mu_B\cdot m_\ell}$$

$\ell = 0, 1, 2, 3, \ldots$

$m_\ell = 0, \pm 1, \pm 2, \ldots \pm \ell$

1.3.3.2. A sugár irányú (radiális) mozgás leírása

Centrális erőtér: $V(\overline{r}) = V(r)$ (1.3.3.1)

$$\left.\begin{aligned} \hat{H}\Psi &= E\Psi \\ \hat{L}^2 Y &= L^2 Y \end{aligned}\right\} \quad \Psi(r,\vartheta,\varphi) = R(r)\cdot Y(\vartheta,\varphi)$$

$$\left(\frac{1}{2m}\hat{p}_r^2 + \frac{1}{2mr^2}\hat{L}^2 + V(r)\right) R\cdot Y = E\cdot R\cdot Y$$

$$Y\cdot\frac{1}{2m}\hat{p}_r^2 R + R\frac{1}{2mr^2}\underbrace{\hat{L}^2\cdot Y}_{L^2 Y} + V\cdot R\cdot Y = E\cdot R\cdot Y \quad \Big|\cdot\frac{1}{Y}$$

$$\boxed{\left[\frac{1}{2m}\hat{p}_r^2 + \underbrace{\left(\frac{L^2}{2mr^2} + V(r)\right)}_{V_{eff}(r)}\right] R = E\cdot R}$$

$L^2 = \hbar^2\,\ell(\ell+1)$

$\ell = 0, 1, 2, 3, \ldots$

59 Láttuk, hogy:

$$\hat{p}_r^2 \equiv -\hbar^2 \Delta_r$$

$$\Delta_r \equiv \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)$$

matematika:

$$\Delta_r R = \frac{1}{r^2}\frac{d}{dr}\underbrace{\left(r^2 \frac{dR}{dr}\right)}_{2rR' + r^2R''} = \frac{2}{r}R' + R''$$

legyen: $P(r) \equiv r \cdot R(r) \longrightarrow P'' = 2R' + rR''$

$\rightarrow$ $P'' = r \cdot \Delta_r R$

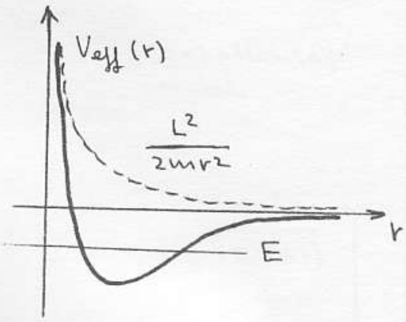
Tehát:

$$-\frac{\hbar^2}{2m}\Delta_r R + V_{eff}\cdot R = E \cdot R \qquad \Big|\cdot r$$

$$-\frac{\hbar^2}{2m}\underbrace{r\Delta_r R}_{P''} + V_{eff}\cdot \underbrace{rR}_{P} = E\cdot \underbrace{rR}_{P}$$

azaz

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V_{eff}(r)\right)P = EP}$$



$$V_{eff}(r) = \frac{L^2}{2mr^2} + V(r)$$

$$L^2 = \hbar^2 \ell(\ell+1) \qquad \ell = 0,1,2,\dots$$

Tetszőleges centrális erőtérben mozgó részecske állapota

$$\Psi(\vec{r}) = \Psi(r,\vartheta,\varphi) = R(r)\cdot P_\ell^{|m_\ell|}(\cos\vartheta)\cdot e^{jm_\ell\varphi}$$

$$L = \hbar\sqrt{\ell(\ell+1)} \qquad \ell = 0,1,2,\dots$$

$$L_z = \hbar m_\ell \qquad m_\ell = 0 \pm 1 \pm 2 \pm \dots \pm \ell$$

$$V(r) \longrightarrow E, R(r)$$

legfontosabb feladatok:

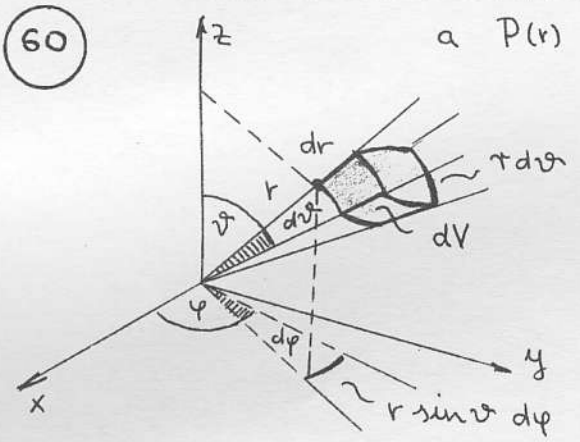
$$V(r) = \frac{1}{4\pi\varepsilon_0}\frac{Q(-e)}{r}$$ (elektron az atomban)

(Feladat)

$$V(r) = \frac{1}{2}m\omega^2 r^2$$ (térbeli harmonikus oszcillátor)

$$V(r) = \begin{cases} 0 & r < r_0 \\ V_0 & r \geq r_0 \end{cases}$$ (gömb alakú potenciál völgy ↓ doboz)

a $P(r)$ fizikai jelentése

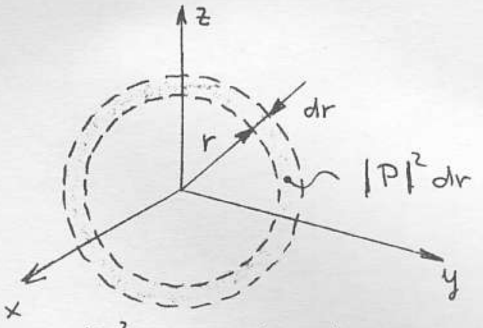


az elemi térfogat:

$$dV = r^2 \sin\vartheta \, d\vartheta \, d\varphi \, dr$$

$$|\psi|^2 dV = \underbrace{|rR|^2 dr}_{(r)} \; \underbrace{|Y|^2 \sin\vartheta \, d\vartheta \, d\varphi}_{(\vartheta,\varphi)}$$

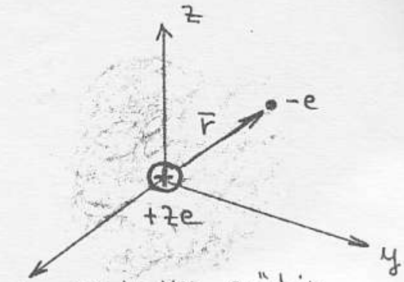
$$|\psi|^2 dV \to \underbrace{|P|^2 dr}_{\downarrow} \cdot \underbrace{\int_0^{2\pi} d\varphi \int_0^{\pi} |Y|^2 \sin\vartheta \, d\vartheta}_{\text{állandó} \equiv 1}$$



$$\int_0^{\infty} |P|^2 dr = 1$$

$|P|^2 dr$ valószínűséggel található a részecske az r sugarú dr vastagságú gömbhéjban $\longrightarrow$ a "centrumtól r távolságra van"

1.3.3.3. A hidrogén szerű ion (a hidrogén atom)



centrális erőtér

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0} \cdot \frac{1}{r} \quad \text{(COULOMB potenciál)}$$

$Z = 1$ (a hidrogén atom)

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

$$\psi(r,\vartheta,\varphi) = \underbrace{R(r)}_{\downarrow} \; \underbrace{Y(\vartheta,\varphi)}_{\text{Gömbfüggvény } (\ell, m_\ell)}$$

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \underbrace{\left(\frac{L^2}{2mr^2} - \frac{Ze^2}{4\pi\varepsilon_0} \frac{1}{r} \right)}_{V_{eff}(r)} \right] P = EP$$

Megoldása: polinom módszerrel

$L^2 = \hbar^2 \ell(\ell+1)$

$\ell = 0, 1, 2, 3, 4, \ldots$

$$\left\{ \begin{array}{l} P_{n,\ell}(r) \quad \text{(LAGUERRE)} \\ E_n = -Z^2 \dfrac{E_0}{n^2} \\ n = 1, 2, 3, \ldots \quad \text{FŐ kvantum szám} \\ \ell = 0, 1, 2, 3, 4, \ldots (n-1) \end{array} \right.$$

$$\left\{ \begin{array}{ll} E_n = \text{állandó}, & L \le L_{max} \\ & \ell \le (n-1) \end{array} \right\} \xleftarrow[\text{FIZIKA}]{}$$

(61) A teljes megoldás hidrogénszerű ion esetén:

$$\boxed{\begin{array}{lll}\psi(r,\vartheta,\varphi) = \frac{1}{r} P_{n,\ell}(r) \cdot P_\ell^{|m_\ell|}(\cos\vartheta) \cdot e^{j m_\ell \varphi} & & \\ E_n = -Z^2 \frac{E_0}{n^2} & n = 1,2,3,\dots & \\ L = \hbar\sqrt{\ell(\ell+1)} & \ell = 0,1,2,\dots,(n-1) & \\ L_z = \hbar m_\ell & m_\ell = 0, \pm 1, \pm 2, \dots \pm \ell & \end{array}}$$

FŐ kvantumszám

MELLÉK ~

MÁGNESES ~

$E_0 = 13{,}6$ eV (a Hidrogén atom ionizációs energiája)

$Z = 1$ (Hidrogén atom esetén)

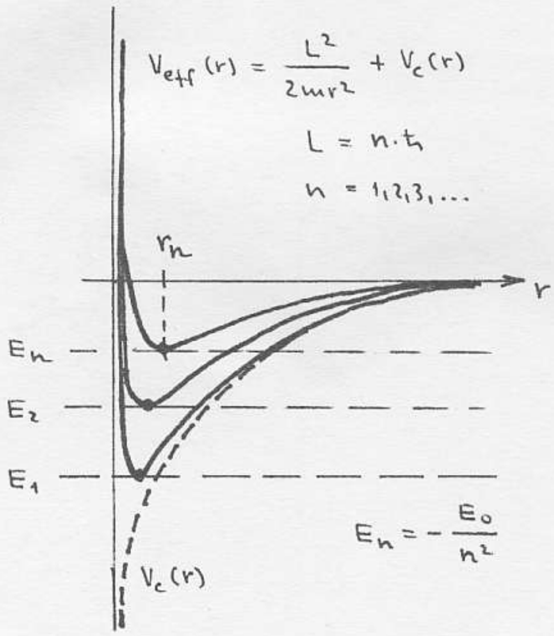
A BOHR modell és a SCHRÖDINGER modell összehasonlítása (H atom)

BOHR

$$V_{eff}(r) = \frac{L^2}{2mr^2} + V_c(r)$$

$$L = n \cdot \hbar$$

$$n = 1,2,3,\dots$$

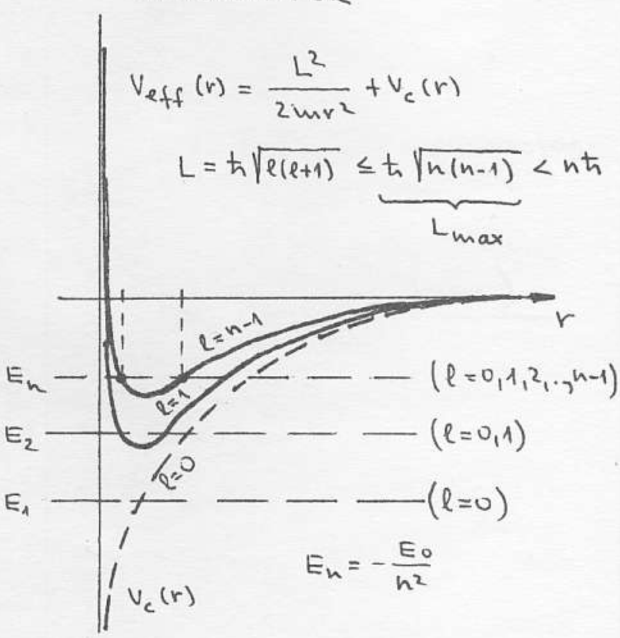


$$E_n = -\frac{E_0}{n^2}$$

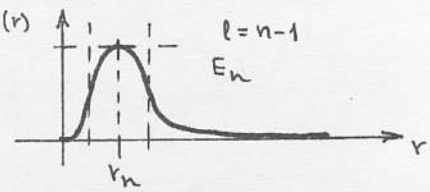
SCHRÖDINGER

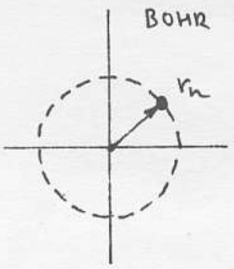
$$V_{eff}(r) = \frac{L^2}{2mr^2} + V_c(r)$$

$$L = \hbar\sqrt{\ell(\ell+1)} \le \underbrace{\hbar\sqrt{n(n-1)}}_{L_{max}} < n\hbar$$

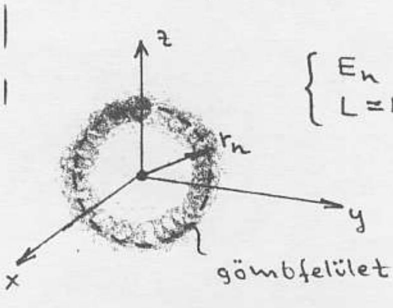


$$E_n = -\frac{E_0}{n^2}$$





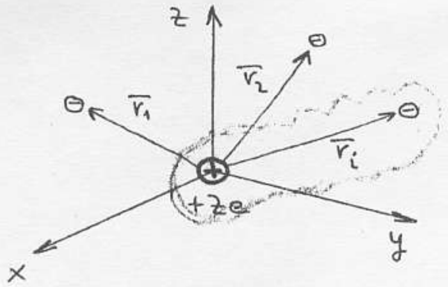
$$\left\{\begin{array}{l} E_n \\ L = L_{max} = n \cdot \hbar \end{array}\right. \quad \leftarrow$$



$$\left\{\begin{array}{l} E_n \\ L = L_{max} = \hbar\sqrt{n(n-1)} \end{array}\right.$$

[Feladatok]

(62) 1.3.3.4. Az atomok elektronszerkezete



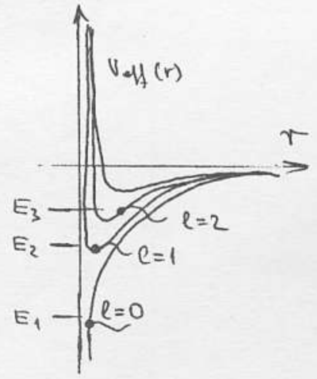
$i = 1, 2, 3, \ldots Z$

Az elektronok közötti kölcsönhatást elhanyagoljuk!

$\psi(\overline{r_i})$ H szerű ion állapot

$\hat{H}\psi = E_n \psi$

$$\boxed{\begin{aligned} \psi_{n,l,m_l} &= R_{n,l}(r)\, P_l^{|m_l|}(\cos\vartheta)\, e^{j m_l \varphi} \\ E_n &= -Z^2 \frac{E_0}{n^2} \qquad n = 1,2,3,\ldots \\ L &= \hbar\sqrt{l(l+1)} \qquad l = 0,1,2,\ldots (n-1) \\ L_z &= \hbar m_l \qquad m_l = 0, \pm 1, \pm 2, \ldots \pm l \end{aligned}}$$



HÉJ →

	s	p			d				
n=4	0 ⊗	−1	0	+1					
n=3	0 ● ×	−1 × ×	0 × ×	+1 × ×	−2	−1	0	+1	+2
n=2	0 ● ●	−1 ● ●	0 ● ●	+1 ● ●					
n=1	0 ● ●								
	s, l=0	ALHÉJ p, l=1			(2l+1) db ALHÉJ d, l=2				

PAULI elv

degeneráció

$$d = 2\sum_{l=0}^{n-1}(2l+1) = 2n^2$$

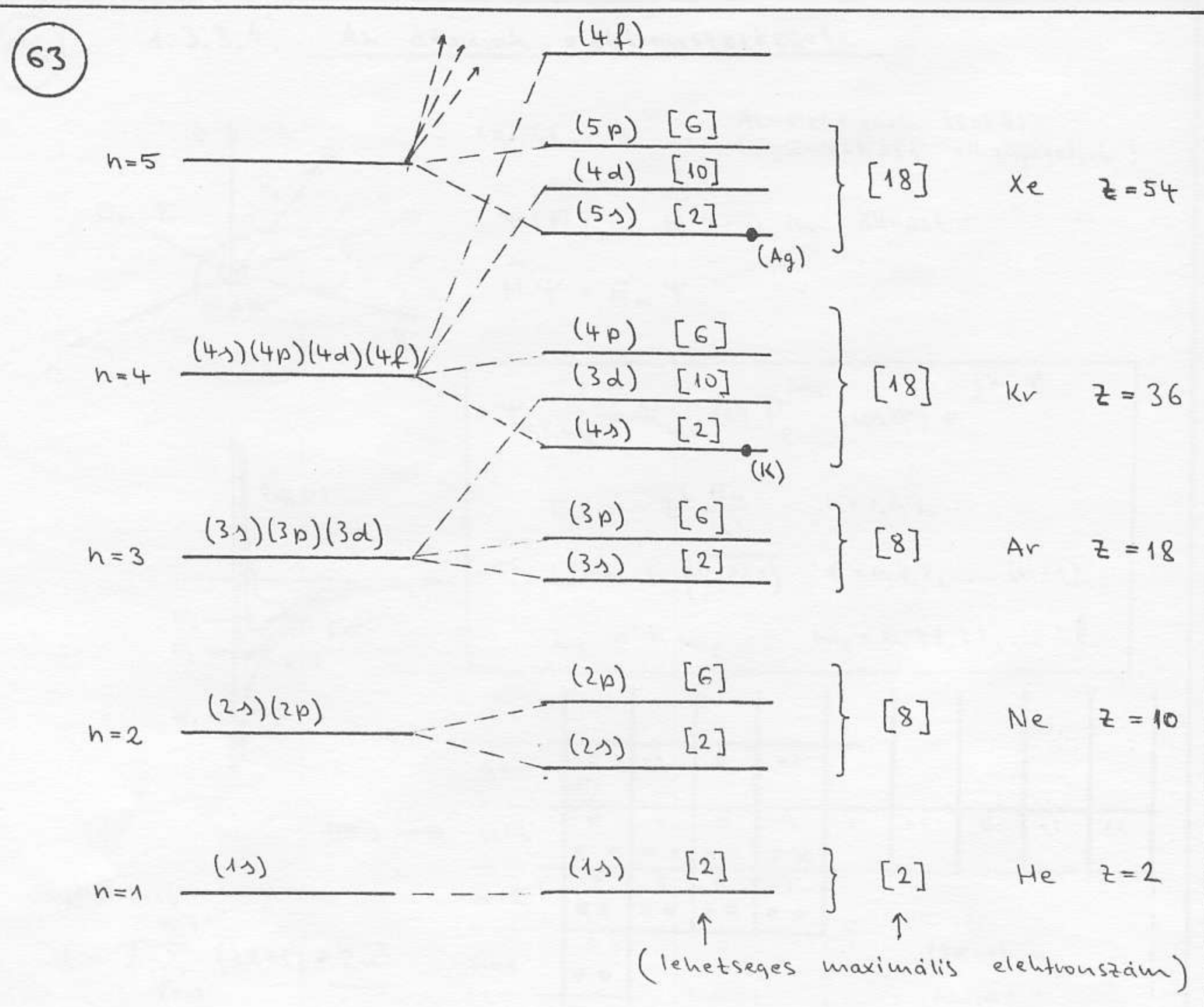
Pl: Na : $(1s)^2(2s)^2(2p)^6(3s)$ $(Z=11)$

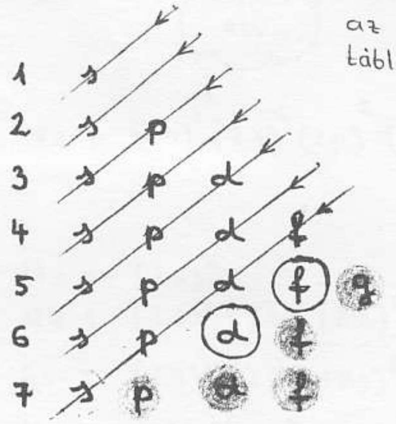
$Z=2$	He :	$(1s)^2$
$Z=10$	Ne :	$(1s)^2\,\underline{(2s)^2(2p)^6}$
$Z=18$	Ar :	$(1s)^2(2s)^2(2p)^6\,\underline{(3s)^2(3p)^6}$
$Z=19$	K :	$[Ar](4s)$ → (3d helyett!)
$Z=36$	Kr :	$[Ar](3d)^{10}\,\underline{(4s)^2(4p)^6}$

↓

Miért ilyen a nemesgázok elektronszerkezete (?)

az elektronok közötti kölcsönhatás nem hanyagolható el.





az alhéjak betöltési sorrendjét megadó táblázat.

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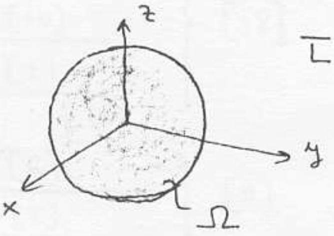
1.3.3.5. Az állapotfüggvények (atompályák) grafikus ábrázolása

s állapotok:

$$\left.\begin{matrix} n \\ \ell = 0 \\ m_\ell = 0 \end{matrix}\right\} P_0^0(\cos\vartheta) = \text{állandó} \quad \left.\right\} \underbrace{\psi_{n,0,0} = R_{n,0}(r)}_{\text{gömbszimmetrikus}}$$

Ábrázolás:

$$\int_\Omega |\psi_{n,0,0}|^2 \, dV \cong 0{,}9$$



$\overline{L} = 0$

s állapot

p állapotok:

$$\left.\begin{matrix} n \\ \ell = 1 \\ m_\ell = 0, \pm 1 \end{matrix}\right\} P_1^{|m_\ell|}(\cos\vartheta) \begin{matrix} \nearrow P_1^0 = \cos\vartheta \\ \searrow P_1^1 = \sin\vartheta \end{matrix}$$

$$\psi_{n,1,-1} = R_{n,1}(r) \cdot \sin\vartheta \cdot e^{-j\varphi}$$

$$\psi_{n,1,0} = R_{n,1}(r) \cos\vartheta$$

$$\psi_{n,1,-1} = R_{n,1}(r) \sin\vartheta \cdot e^{+j\varphi}$$

láttuk, hogy: $\hat{L}^2 = -\hbar^2 \Delta_\vartheta + \frac{1}{\sin^2\vartheta} \hat{L}_z^2$

$$\left\{\begin{matrix} \hat{L}^2 Y = L^2 Y \\ \hat{L}_z^2 \Phi = L_z^2 \Phi \end{matrix}\right. \longrightarrow \left.\begin{matrix} \Phi = e^{\pm j |m_\ell| \varphi} \\ L_z^2 = \hbar^2 m_\ell^2 \end{matrix}\right] \text{degenerált állapot}$$

lineáris kombinációval ($m_\ell = \pm 1$ esetén)

$$\{e^{-j\varphi}, e^{+j\varphi}\} \rightarrow \{\sin\varphi, \cos\varphi\}$$

(Feladat: bizonyítás)

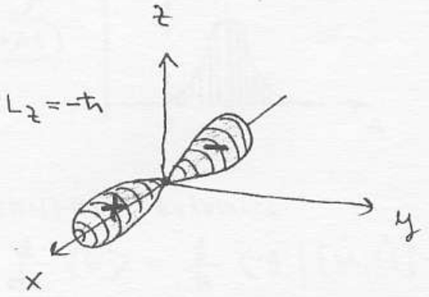
65 Legyen

$$\psi_{n,1,-1} = R_{n,1}(r)\sin\vartheta \cdot \cos\varphi$$
$$\psi_{n,1,0} = R_{n,1}(r)\cos\vartheta$$
$$\psi_{n,1,1} = R_{n,1}(r)\sin\vartheta\,\sin\varphi$$

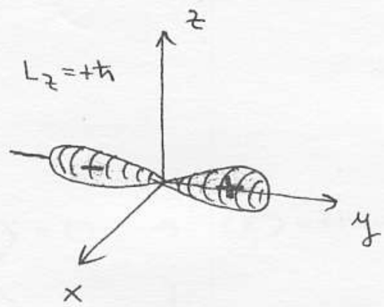
Polár (gömbi) koordináták definíciója

$$x = r\sin\vartheta\cos\varphi$$
$$y = r\sin\vartheta\sin\varphi$$
$$z = r\cos\vartheta$$

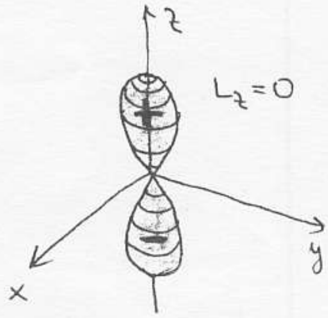
$$\rightarrow \boxed{\begin{aligned}\psi_{n,1,-1} &= R_{n,1}\frac{x}{r}\\ \psi_{n,1,0} &= R_{n,1}\frac{z}{r}\\ \psi_{n,1,+1} &= R_{n,1}\frac{y}{r}\end{aligned}}$$



$\psi_{n,1,-1} \rightarrow p_x$ állapot



$\psi_{n,1,+1} \rightarrow p_y$ állapot



$\psi_{n,1,0} \rightarrow p_z$ állapot