$\rightarrow \langle \vartheta, \varphi | lm \rangle = Y_{lm}(\vartheta, \varphi)$

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

$L_z \psi_{lm}(\vec{r}) = \hbar m \psi_{lm}(\vec{r})$ → ψ je tudi rešitev Schrödingerjeve enačbe:
$\hat{H}\psi = E\psi$
→ torej je ψ periodična v kotu → $\psi(\varphi) = \psi(\varphi + 2\pi)$

$-i\hbar \frac{\partial}{\partial \varphi}\psi(\varphi) = \hbar m \psi(\varphi)$

$\psi = C e^{im\varphi} = C e^{im(\varphi + 2\pi)}$

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

Pogoj periodičn. ← $\boxed{m \in \mathbb{Z}}$

sledi, da mora biti tudi $l \in \mathbb{N}$

Primer: $f(\vartheta, \varphi) = \sqrt{\sin\vartheta}\, e^{i\frac{\varphi}{2}}$

$L^2 f = \xi f$
→ nima celoštevilčnega m-ja
ta ni enolična rešitev, $m \notin \mathbb{Z}$
To je zato..

Kaj je pa zdaj s tistimi polovicami na prejšnji strani? ←

→ Tam nismo upoštevali, da so rešitve Schröd. enačbe in nismo imeli pogoje enoličnosti /periodičnosti.

Ko bomo prišli do operatorje spina, ne bomo sploh govorili o krajevnem delu funkcije in ne bo pogoja enoličnosti. Bo le gor ali dol. Tam bo lahko polovično...

Centralni potencial

→ $V(\vec{r}) = V(r)$

Klasično: $\vec{L} = \vec{r} \times \vec{p} = \vec{r} \times m\dot{\vec{r}}$

$$\dot{\vec{L}} = \cancel{\dot{\vec{r}} \times m\dot{\vec{r}}} + \vec{r} \times m\ddot{\vec{r}} = \vec{r} \times \underbrace{m\ddot{\vec{r}}}_{\vec{F}} = \vec{r} \times \vec{F}(\vec{r})$$

če je $\vec{F}(\vec{r}) = \vec{F}(r)$
oz. $\vec{F} = -\nabla V(r)$

→ $\dot{\vec{L}} = \vec{r} \times (-\nabla V(r)) = \emptyset$ → Vrtilna količina se ohranja. Lušno.

$[L^2, V(r)] = 0$

$[L^2, H] = 0$

$[L_z, H] = 0$

sferične koordinate :

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}\right]$$

$$H\psi_{elm}(\vec{r}) = E\,\psi_{elm}(\vec{r})$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi_{elm} = E\psi_{elm}$$

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{L^2}{2mr^2} + V(r)\right]\psi_{elm} = E\psi$$

→ L^2 se preprosto prepiše v $\hbar^2 l(l+1)$

energije klasično: $\frac{1}{2}mv^2 + \frac{1}{2}J\omega = \frac{p^2}{2m} + \frac{L^2}{2J}$

$L = J\omega$

$J = mr^2$

$$\psi_{elm}(\vec{r}) = R(r)\,Y_{elm}(\vartheta,\varphi)$$

osnovni trik v 3D :

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

v 2D: $R(r) = \frac{u}{\sqrt{r}}$

normalizacije: $\int_0^\infty \frac{u^2}{\cancel{r^2}}\cancel{r^2}dr$ to se pokrajša

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

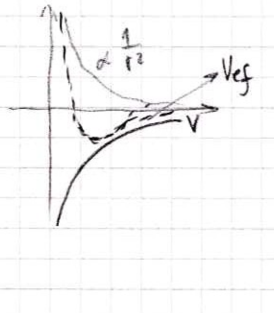
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(ru' - u\right) = \frac{1}{r^2}\left(u' + ru'' - u'\right) = \frac{u''}{r}$$

torej Schrö. enačba preide v obliko:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V_{ef}(r)\right]u(r) = E\,u(r)$$ → enodim. problem je rešen, znamo mi to.

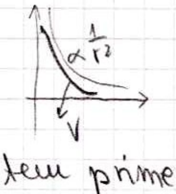
$$V_{ef}(r) = V(r) + \underbrace{\frac{\hbar^2 l(l+1)}{2mr^2}}_{}$$ → popravljen potencial

"odbojni" potencial, klasično bi bila to centrifugalna sila...



V(r)

a) $r \to 0$ $|V| \leq \frac{1}{r^2}$



$r^2|V| \to 0$ ko $r \to 0$.

v tem primeru lahko za male r zanemarimo člen V(r) v primerjavi z $\frac{\hbar^2 l(l+1)}{2mr^2}$. Potencial je tam, ampak je kot da ga ni. Rešitve so Besseli in Neumann. ↗

b) $r \to \infty$

če $V(r)$ dovolj hitro pada, lahko zopet potencial zanemarimo. In so rešitve eksponentne funkcije.

$$H\psi_{lm} = E\psi_{lm}$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(r)\right)\psi_{lm} = E\psi_{lm}$$

$$\left[\overbrace{-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)} + \frac{\overset{\nearrow \hbar^2 l(l+1)}{L^2}}{2mr^2} + V(r)\right]\psi_{lm} = E\psi$$

$$p^2$$

$$\left[\frac{p^2}{2m} + \frac{L^2}{2J} + V(r)\right]\psi_{lm} = E\psi_{lm}$$

$$\psi_{lm}(\vec{r}) = R(r)Y_{lm}(\vartheta,\varphi)$$

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

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\left(\frac{u}{r}\right)\right) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\,\frac{u_r\cdot r - u}{r^2}\right) = \frac{1}{r^2}\left(u_{rr}r + u_r - u_r\right) =$$

$$= \frac{u_{rr}}{r} = \frac{1}{r}\frac{\partial^2 u}{\partial r^2}$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V_{eff}(r)\right]u(r) = Eu$$

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

Komentar:

a) $r \to 0 \quad |V| \ll \frac{1}{r^2} \Rightarrow r^2|V| \to 0$

rešitev je takšna, kot da ni potenciala; prevlada $\frac{L^2}{2mr^2}$; rešitve so Besselove in Neumannove f.

b) $r \to \infty$, če lahko zanemarimo, so rešitve eksponentne funkcije

To je Schrödinger ponoči izpeljal. Kako se pa to ve! Strnada se vpraša. Kako pa on ve! On ga je gledal

Akta

A je kakina kuga?

$V(\vec{r}) = V(r)$

$\Psi(r,\vartheta,\varphi) = \frac{u(r)}{r} Y_{lm}(\vartheta,\varphi)$

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

$V_{ef} = V(r) + \frac{\hbar^2(l+1)l}{2mr^2}$

Če je energija omejena nemoremo imeti velikih l pri majhnih r.

a) Če $V(r) - E \ll \frac{1}{r^2}$ $(r \to 0)$

$u(r) = A \cdot r^{\alpha}$

$-\alpha(\alpha-1) r^{\alpha-2} + l(l+1) r^{\alpha-2} = 0$

$\alpha(\alpha-1) = l(l+1)$

$\alpha = l+1$
$\alpha = -l$

$u(r) = \left(A r^{l+1} + B r^{-l}\right)\left(1 + \mathcal{O}(r)\right)$

$\to l = 0 \Rightarrow u(r) = Ar + B$ (pravilna rešitev $c_1 \sin\varkappa r + c_2 \cos\varkappa r$)

b) $r \to \infty$

$\frac{V_{ef}}{|E|} \to 0$

$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - E\right) u = 0$

$E = -\frac{\hbar^2\varkappa^2}{2m} \Rightarrow \left(-\frac{d^2}{dr^2} + \varkappa^2\right) u = 0 \Rightarrow u = A e^{-\varkappa r} + B e^{\varkappa r}$

* * *

$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - \frac{e_0^2 Z}{4\pi\varepsilon_0 r} + \frac{\hbar^2 l(l+1)}{2mr^2}\right] u(r) = E\, u(r)$

$u \sim e^{-\rho}$ $\quad \rho = \varkappa r$; $\frac{\hbar^2}{2m} = \frac{|E|}{\varkappa^2}$

$$\left[+\frac{d^2}{d\rho^2}-\frac{l(l+1)}{\rho^2}+\frac{\rho_0}{\rho}-1\right]u(\rho)=0$$

$$\rho_0=\frac{e_0^2\, \varkappa}{4\pi\varepsilon_0\, |E|}$$

$$u(\rho)=\rho^{l+1}e^{-\rho}w(\rho)$$

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

$$=(l+1)l\rho^{l-1}e^{-\rho}w(\rho)+(l+1)\rho^{l}(-1)e^{-\rho}w(\rho)+$$

$$+(l+1)\rho^{l}\cancel{e}^{-\rho}w'(\rho)+(l+1)\rho^{l}(-1)e^{-\rho}w(\rho)+\rho^{l+1}e^{-\rho}w(\rho)+$$

$$+\rho^{l+1}(-1)e^{-\rho}w'(\rho)+(l+1)\rho^{l}\cancel{e}^{-\rho}w'(\rho)+\rho^{l+1}\cancel{(-1)}e^{-\rho}w'(\rho)+$$

$$+\rho^{l+1}\cancel{e}^{-\rho}w''(\rho)=$$

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

$$\rho\frac{d^2w}{d\rho^2}+2(l+1-\rho)\frac{dw}{d\rho}+(\rho_0-2(l+1))w=0$$

$$w(\rho)=\sum_{k=0}^{\infty}a_k\rho^k$$

$$\sum_{k=0}^{\infty}a_k\left[k(k-1)\rho^{k-1}+2(l+1)k\rho^{k-1}-2k\rho^k+(\rho_0-2(l+1)\rho^k\right)=0$$

$$\sum_{j=-1}^{\infty}a_j\left[(j+1)j\rho^j+2(l+1)(j+1)\rho^j\right]+\sum_{k=0}^{\infty}a_k\left[-2k\rho^k+(\rho_0-2(l+1))\rho^k\right]=0$$

Pri $j=-1\Rightarrow$ 1. člen $=0$

$$\sum_{k=0}^{\infty}\left[a_{k+1}\left((k+1)k+2(l+1)(k+1)\right)+a_k\left(-2k\cancel{\rho}+(\rho_0-2(l+1))\right)\right]\rho^k=0$$

$$d_{k+1} = \frac{-2k+\rho_0-2(l+1)}{-k(k+1)-2(l+1)(k+1)}\, d_k$$

$\rho_0 = !$ $\Rightarrow$ ne sme divergirati

$$\frac{d_{k+1}}{d_k} \xrightarrow{k\to\infty} \frac{2}{k} ,$$

$$e^{2x} = \sum_{k=0}^{\infty} \frac{1}{k!}(2x)^k \Rightarrow \frac{2^{k+1}\, k!}{(k+1)!\, 2^k} = \frac{2}{k+1}$$

$$w(\rho) \sim e^{2\rho}$$

$u = \rho^{l+1} e^{-\rho} e^{2\rho} \to e^{\rho}$ Divergira

Da to ne divergira, mora $\exists N$, da so vsi d_n od tam naprej enaki 0.

$$-2N + \rho_0 - 2(l+1) = 0$$

$\rho_0 = 2(N+l+1)$ $\to$ cela števila

$$2(N+l+1) = \frac{e_0^2 Z}{4\pi\varepsilon_0}\cdot\frac{\kappa}{|E|} \qquad \kappa^2 = \frac{|E|}{\hbar^2}\cdot 2m$$

$$E = -\frac{m Z^2 e_0^4}{2\hbar^2(4\pi\varepsilon_0)^2}\,\frac{1}{(N+l+1)^2} = -\frac{E_1 Z^2}{n^2} \qquad E_1 = 13{,}6\ \text{eV}$$

$n \in \mathbb{N}$

$l = n - N - 1$ Od tod sledi: $l = n-1$
$l = n-2$
$\vdots$
$l = 0$

$m = l, l-1, \dots, -l \Rightarrow 2l+1$

E_n je energija elektrona: imamo več valovnih funkcij (degeneracija)

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

Razlog za tako veliko degeneracijo je visoka simetrija. Potencial $\frac{1}{r}$ ima degeneracijo, da energija ni odvisna od l.

Runge - Lenzov vektor je tudi konstanta - kaže v smeri glavne polosi

$$\vec{A} = \frac{1}{2m}\left(\vec{p}\times\vec{L} - \vec{L}\times\vec{p}\right) - \frac{Ze^2\vec{r}}{4\pi\varepsilon_0 r}$$

1. $\vec{A} = \vec{A}^+$
2. $\vec{A}\cdot\vec{L} = \vec{L}\cdot\vec{A} = 0$
3. $[A, H] = 0$ za primer Culombskega potenciala

Če $\vec{A}$ ne bi bil konstanta, bi imeli degeneracijo samo 2l+1.

Lastne funkcije

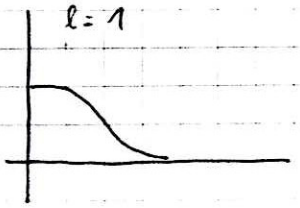
$$\Psi_{nlm}(r,\vartheta,\varphi,t) = e^{-i\frac{E_n}{\hbar}t} R_{nl}(r)\, Y_{lm}(\vartheta,\varphi)$$

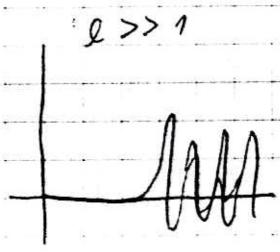
Ker je tako degenerirana, mora biti kompleksna

$$R_{nl}(r) = \frac{u(r)}{r} = -\left[\frac{(n-l-1)!\,(2\kappa)^3}{2n\left((n+l)!\right)^3}\right]^{1/2} (2\kappa r)^l e^{-\kappa r} \underset{\uparrow}{L^{2l+1}_{n+l}}(2\kappa r)$$

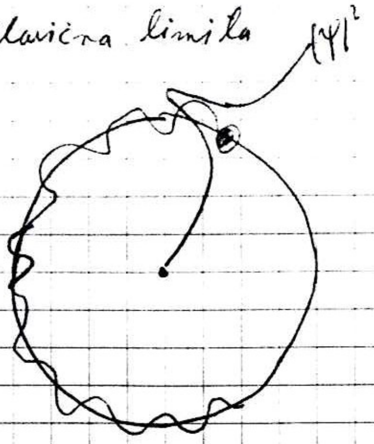
pridruženi Laguerrov polinom

R_{nl} ima n-l-1 ničel

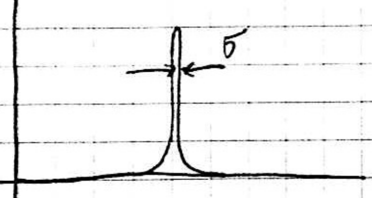




Klasična limita



$\Psi_{n,n-1,n} \sim r^{n-1} e^{-\frac{r}{na}}$ a - Bohrov radij



$\langle r_n\rangle \sim \frac{n^2}{Z}\cdot a$

$\sigma \sim \frac{1}{\sqrt{n}}$

Bohrov model ni znal razložiti, zakaj elektron ne seva. Tudi mi ne znamo.

$$\hbar\omega_{m,n} = E_m - E_n = E_1\left(-\frac{1}{m^2}+\frac{1}{n^2}\right)$$

Dva sosednja nivoja:

$$-\frac{1}{(n+1)^2}+\frac{1}{n^2} = \frac{n^2+2n+1-n^2}{(n+1)^2 n^2} \xrightarrow{n\to\infty} \frac{2}{n^3}$$

$h\cdot\omega = \frac{2E_1}{n^3}$ - energija, ki jo izseva elektron, ko preskoči med visokima sosednjima nivojema.

Ta zadeva ustreza frekvenci kroženja pri Keplerjevem problemu

$\rightarrow \frac{e^2}{4\pi\varepsilon_0 r^2} = \omega^2 m r$; $\hbar n = \omega\cdot m r^2$ → kvantizacija vrtilne količine - zahteva, da se izide valovna dolžina

Nabit delec v magnetnem polju

$\vec{A}, \phi$

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

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

$H = \frac{1}{2m}\left(\vec{p} - e\vec{A}\right)^2 + e\phi$ - klasično

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

$$(\nabla\cdot\vec{A} + \vec{A}\cdot\nabla)\psi = \nabla\cdot\psi\vec{A} + \vec{A}\cdot\nabla\psi = (\nabla\psi)\cdot\vec{A} + \psi\nabla\cdot\vec{A} + \vec{A}\cdot\nabla\psi = 2\vec{A}\cdot\nabla\psi + \psi\nabla\vec{A}$$

Coulombova umeritev: $\nabla\cdot\vec{A} = 0$ - za nas OK, čeprav ni relativistično invariantna

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2\nabla^2}{2m}\psi + \frac{i\hbar e}{m}\vec{A}\cdot\nabla\psi + \frac{e^2}{2m}A^2\psi + e\phi\psi + C\psi\cdot\overset{=0}{\nabla\cdot\vec{A}}$$

Omejimo se na konstantno magnetno polje.

$\vec{B} = \vec{B}_0 =$ konst.

$\vec{A} = -\frac{1}{2}(\vec{r}\times\vec{B}_0) \Rightarrow \nabla\times\vec{A} = \vec{B}_0$

$\vec{\nabla}\cdot\vec{A} = -\frac{1}{2}\vec{\nabla}\cdot(\vec{r}\times\vec{B}_0) = 0 \quad \left(\nabla\cdot(\vec{v}\times\vec{w}) = \vec{v}\cdot(\vec{\nabla}\times\vec{w}) - \vec{w}\cdot(\vec{\nabla}\times\vec{v})\right)$