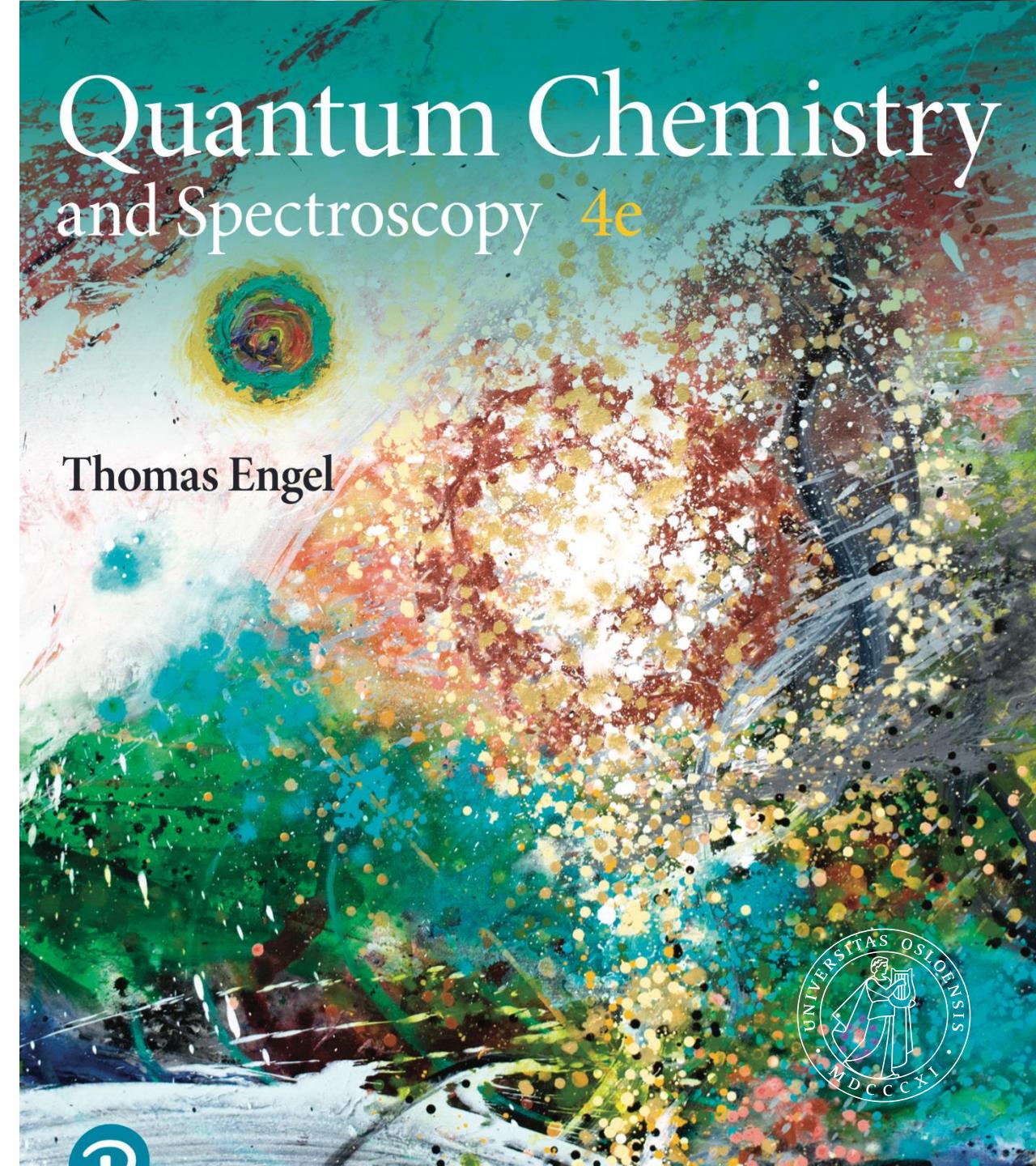


UNIVERSITETET
I OSLO

KJM2601 – forelesning 11

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Hylleraassenteret

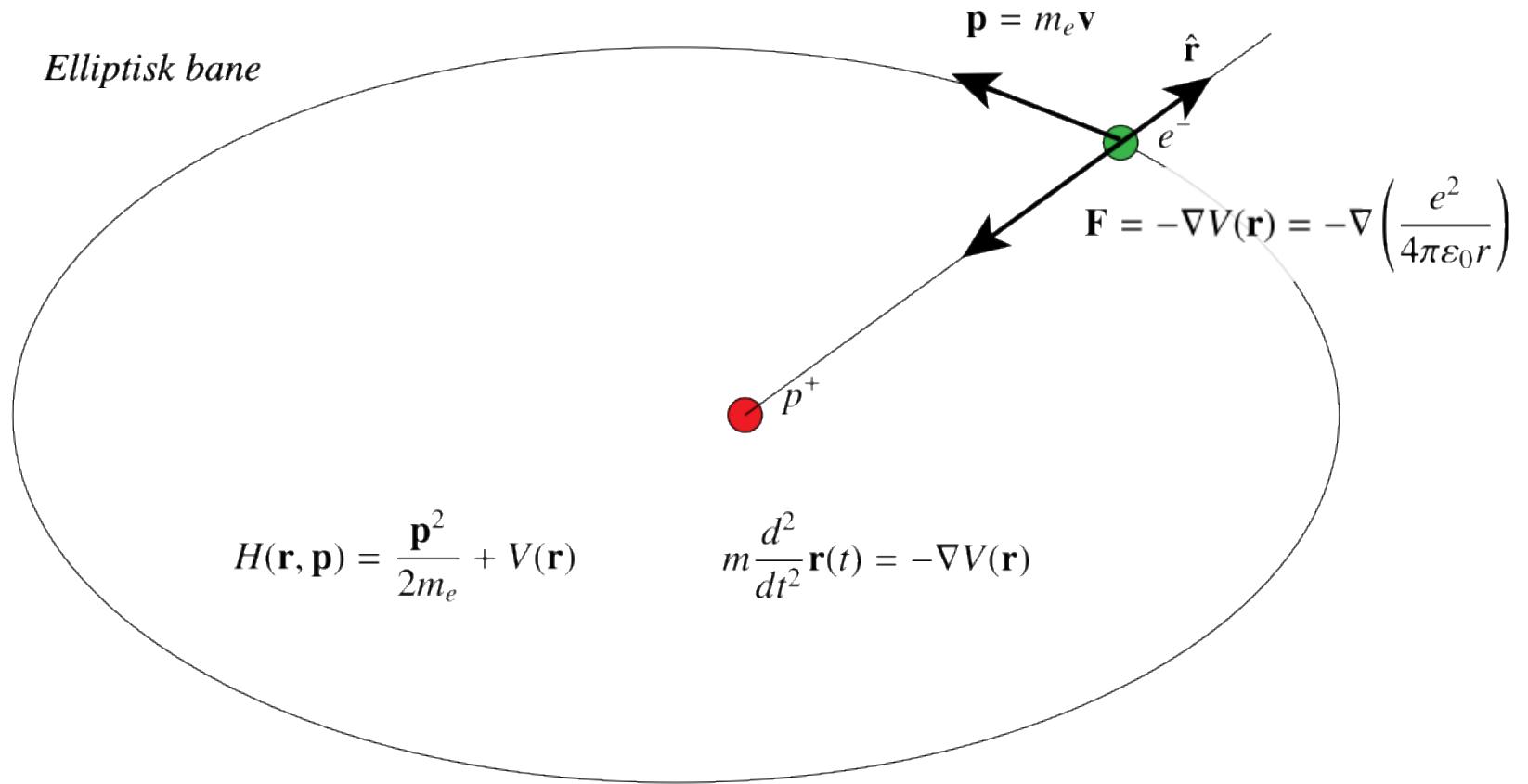
2/10/2024



Hydrogenatomet

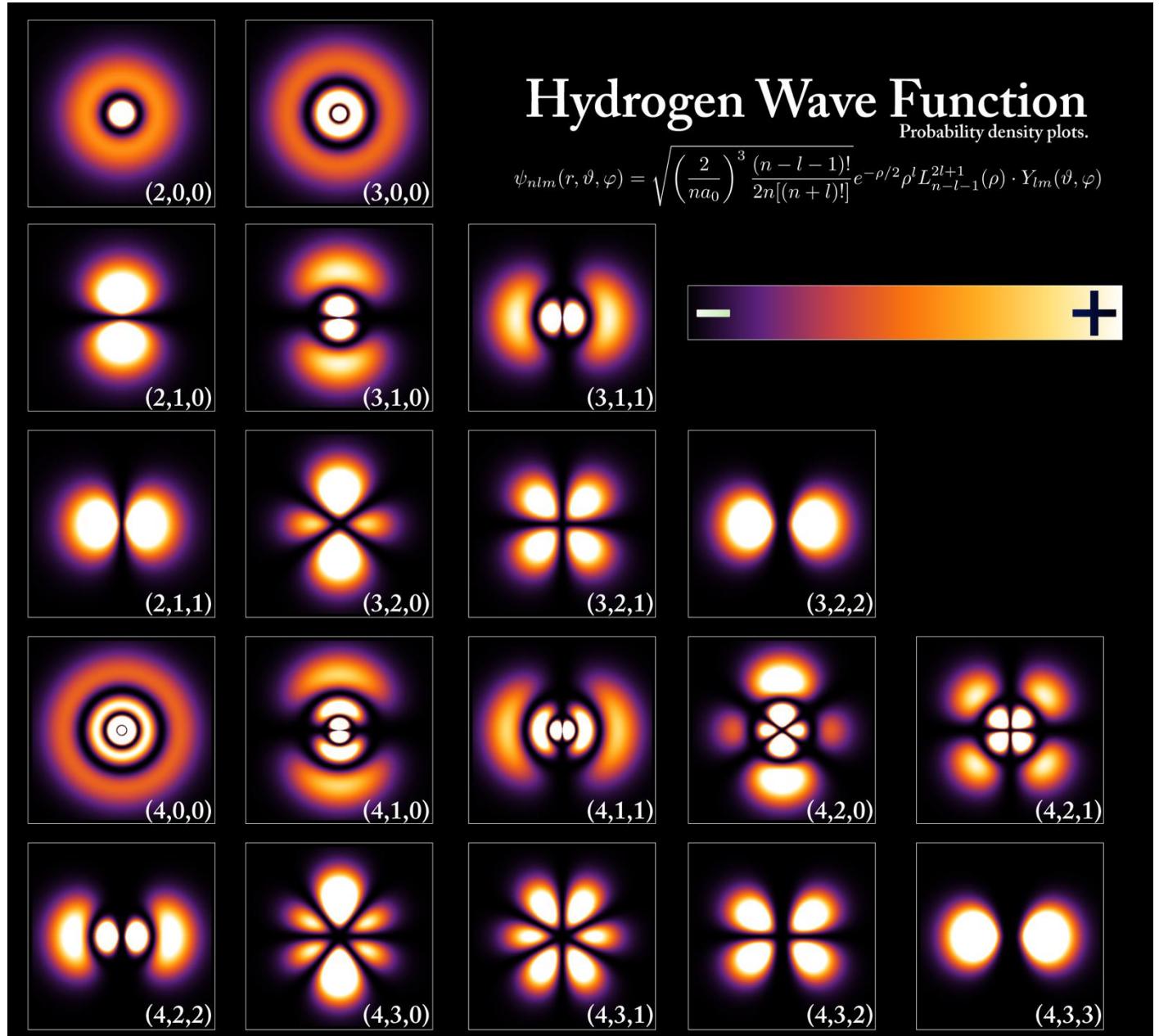
Det klassiske H-atomet

- Veldefinert posisjon, bevegelsesmengde
- Newtons lover
- Periodiske elliptiske baner



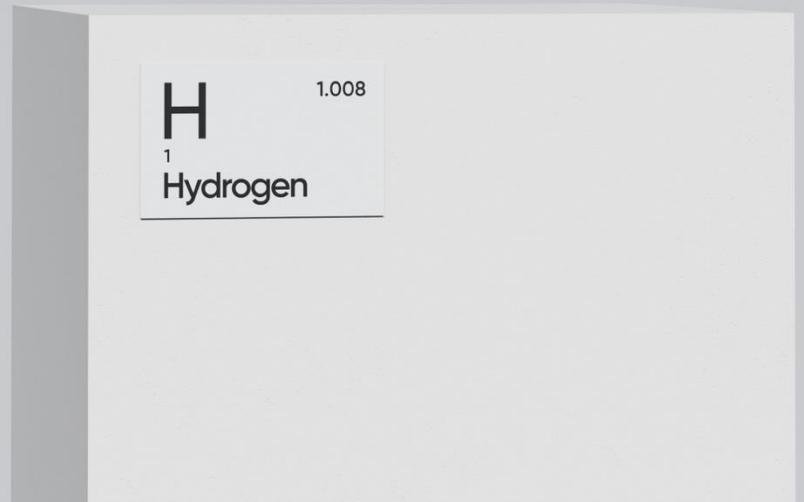
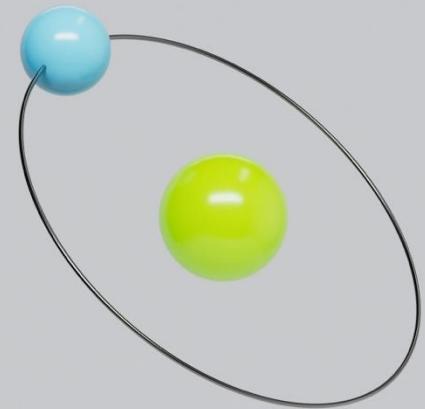
Det kvantemekaniske H-atomet

- Bølgefunksjon
- Schrödingerlikninga
- Egenfunktjoner/stasjonære tilstander



Hvorfor skal vi studere H-atomet?

- Et svært vanlig grunnstoff
- Det eneste atomet der kvantemekanikken kan løses eksakt
- Mye innsikt overførbar til andre atomer



Å løse Schrödingerlikninga

Schrödingerlikninga i kartesiske koordinater

Coulomb-potensialet

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

Kinetisk energi

$$\hat{H} = -\frac{\hbar^2}{2m_e} \nabla^2 - \frac{e^2}{4\pi\epsilon_0} \frac{1}{r}, \quad r = |\mathbf{r}|$$



Dette blir altfor
komplisert ...

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

$$r = |\mathbf{r}| = \sqrt{x^2 + y^2 + z^2}$$

Laplace-operator

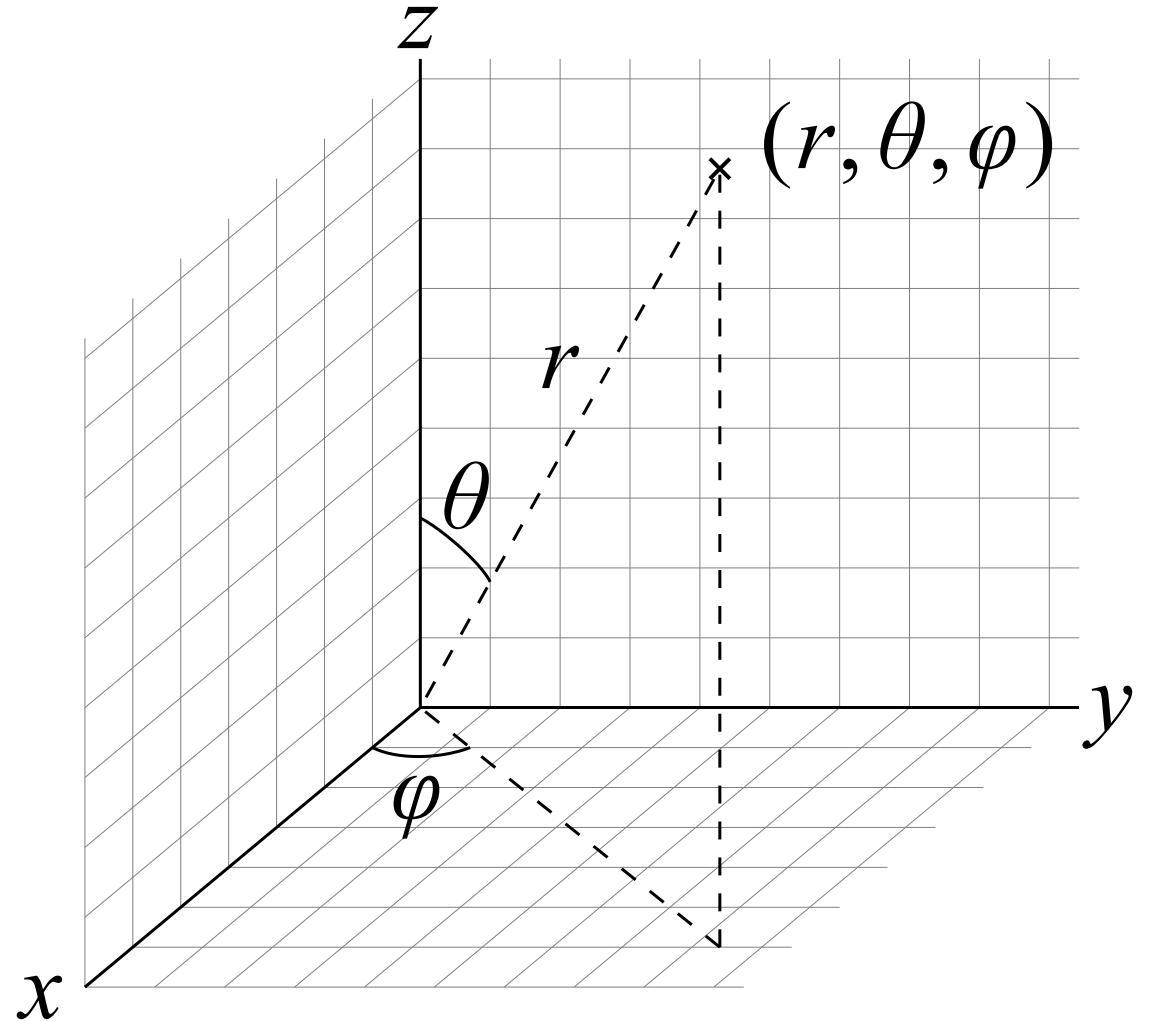
Kulekoordinater

- Vi skal jobbe med kulekoordinater
- Velegnet ved kulesymmetri

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$



Schrödingerlikninga i kulekoordinater

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x} \frac{\partial}{\partial \varphi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial z} \frac{\partial}{\partial \varphi}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y} \frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial y} \frac{\partial}{\partial \varphi}$$

Kjerneregelen. Brukes til
å skrive om Laplace-
operatoren

$$\nabla^2 \psi(r, \theta, \varphi)$$

$$\begin{aligned} & -\frac{\hbar^2}{2m_e} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi(r, \theta, \varphi)}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi(r, \theta, \varphi)}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi(r, \theta, \varphi)}{\partial \varphi^2} \right] \\ & -\frac{e^2}{4\pi\epsilon_0 r} \psi(r, \theta, \varphi) = E\psi(r, \theta, \varphi) \end{aligned}$$

Er dette noe
lettere da ...?

Angulærmoment

$$\begin{aligned} & -\frac{\hbar^2}{2m_e} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi(r, \theta, \varphi)}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi(r, \theta, \varphi)}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi(r, \theta, \varphi)}{\partial \varphi^2} \right] \\ & -\frac{e^2}{4\pi\epsilon_0 r} \psi(r, \theta, \varphi) = E\psi(r, \theta, \varphi) \end{aligned}$$

$$\hat{\ell}^2 \psi(r, \theta, \varphi) = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi(r, \theta, \varphi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi(r, \theta, \varphi)}{\partial \varphi^2} \right]$$

Angulærmoment fra
rigid rotor i 3D !

$$\hat{\ell}^2 Y_l^m(\theta, \varphi) = \hbar^2 l(l+1) Y_l^m(\theta, \varphi)$$

Kuleflatefunksjonene

$$\frac{1}{2m_e} \left[-\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \hat{\ell}^2 + V(r) \right] \psi(r, \theta, \varphi) = E\psi(r, \theta, \varphi)$$

«Ny» SL!

Separasjon av variable

- Hamiltonoperatoren er en sum av to enklere operatorer ...
- Vi prøver med bølgefunksjon på produktform

$$\psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \varphi)$$

- Vi setter inn ...

$$\begin{aligned} & \left[\frac{1}{2m_e} \left(-\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \hat{\boldsymbol{\ell}}^2 \right) + V(r) \right] R(r) Y_l^m(\theta, \varphi) \\ &= \left[\frac{1}{2m_e} \left(-\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{\hbar^2 l(l+1)}{r^2} \right) + V(r) \right] R(r) Y_l^m(\theta, \varphi) = ER(r) Y_l^m(\theta, \varphi) \quad (1) \end{aligned}$$

- Vi dividerer på kuleflatefunksjonen og får radiallikningen:

$$\left[\frac{\hbar^2}{2m_e} \left(-\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) + V(r) \right] R(r) = ER(r)$$



Sentrifugalkrefter

- Vi introduserer et effektivt potensial

$$V_{\text{eff}}(r) = \frac{\hbar^2}{2m_e} \frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0 r}$$



Sentrifugalterm

Coulomb

- For ulike l vil vi få ulike radialfunksjoner $R(r)$
- Men m har ingenting å si !

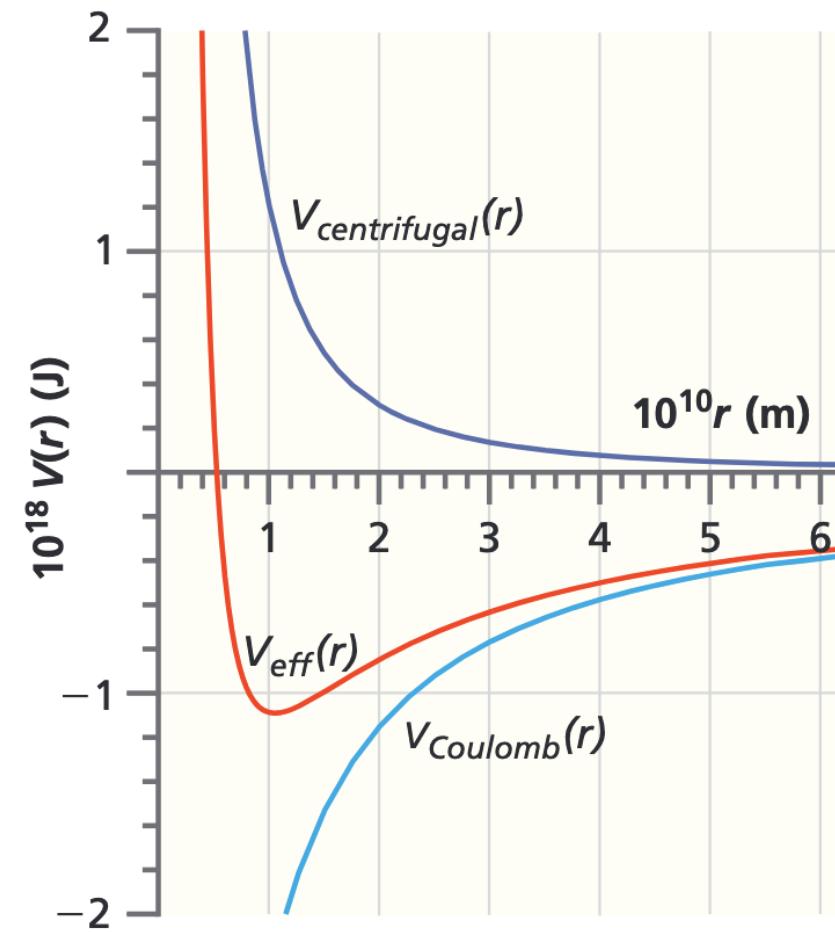


Figure 9.1

Individual contributions to the effective potential and their sum plotted as a function of distance. The centrifugal potential used is for $l = 1$; larger values of l make the effective potential more repulsive at small r .

Egenverdiene

- Vi skal nå se på løsningene av radiallikningen:

$$\left(-\frac{\hbar^2}{2m_e} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + V_{\text{eff}}(r) \right) R_{n,l}(r) = E_{n,l} R_{n,l}(r)$$

- Det viser seg at energiene ikke avhenger av l :

$$E_{n,l} = E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2 n^2} \approx -\frac{13.6 \text{ eV}}{n^2}, \quad \text{for } n = 1, 2, 3, 4, \dots$$

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

Krever detaljert analyse for å vise ...

- Dersom $V(r)$ ikke var Coulomb, men noe annet, så ville energiene også avhengt av l .

Eksperimentell evidens

- H-spekter har vært observert siden 1885
- Bohrs modell klarte å «forklare» spekteret
- Men Schrödinger gav komplett modell
 - Ad hoc kvantiseringshypotese borte
 - I prinsippet anvendbart på all materie
- At bølgemekanikken skulle gjenvinne dette og mer til er intet mindre enn mirakuløst!



- (Men hva med He-atomet, eller molekyler med >1 elektron?)

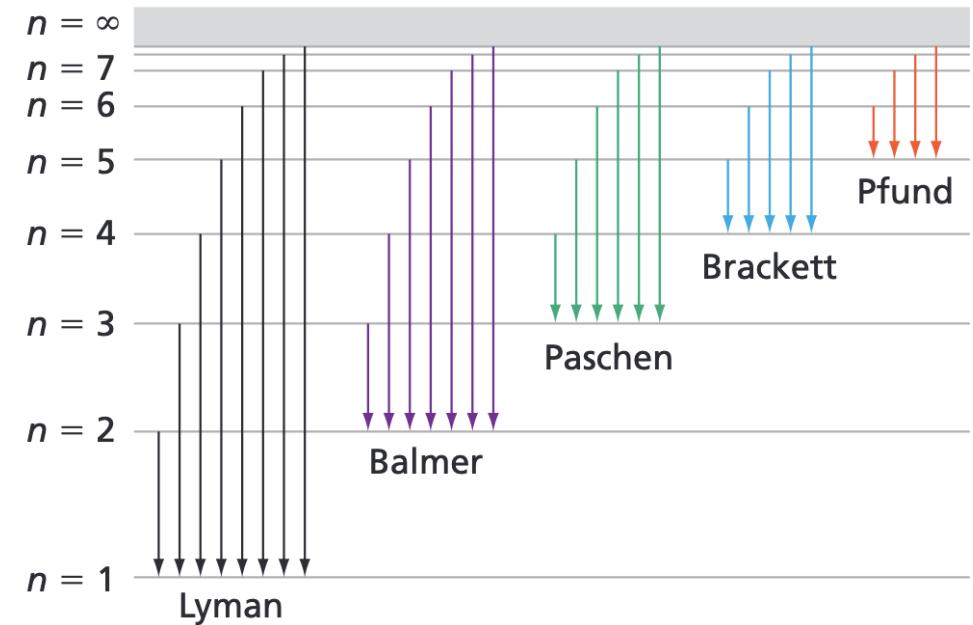


Figure 9.3

Energy-level diagram for the hydrogen atom showing allowed transitions for $n < 8$. Because energy levels are continuous for $E > 0$, the absorption spectrum is continuous above an energy that depends on the initial n value, as indicated by the gray area. The different sets of transitions are named after the scientists who first investigated them.

Degenerasjon: flere egenfunksjoner per egenverdi

- Egenverdiene kan ikke avhenge av m ...

$$m = \underbrace{-l, -l+1, -l+2, \dots, l-1, l}_{2l+1 \text{ muligheter}}$$

- Så det er $2l+1$ egenfunksjoner for hver $E_{n,l}$.
- Egenverdiene avhenger ikke av l heller, total degenerasjonsgrad

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

E_n	nl	m	g_n
E_1	1s	0	1
E_2	2s	0	
	2p	-1, 0, 1	4
E_3	3s	0	
	3p	-1, 0, 1	9
	3d	-2, -1, 0, 1, 2	
E_4	4s	0	
	4p	-1, 0, 1	16
	4d	-2, -1, 0, 1, 2	
	4f	-3, -2, -1, 0, 1, 2, 3	

Spektroskopisk
notasjon

Radialfunksjonene

$$R_{nl}(r) = (\text{polynom av grad } n - 1) \times \exp[-r/(a_0 n)] \quad a_0 = \frac{\varepsilon_0 h^2}{\pi m_e e^2} \approx 0.529 \times 10^{-10} \text{ m} = \text{Bohr radius}$$

$$n = 1, l = 0 \quad R_{10}(r) = 2 \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}$$

$$n = 2, l = 0 \quad R_{20}(r) = \frac{1}{\sqrt{8}} \left(\frac{1}{a_0} \right)^{3/2} \left(2 - \frac{r}{a_0} \right) e^{-r/2a_0}$$

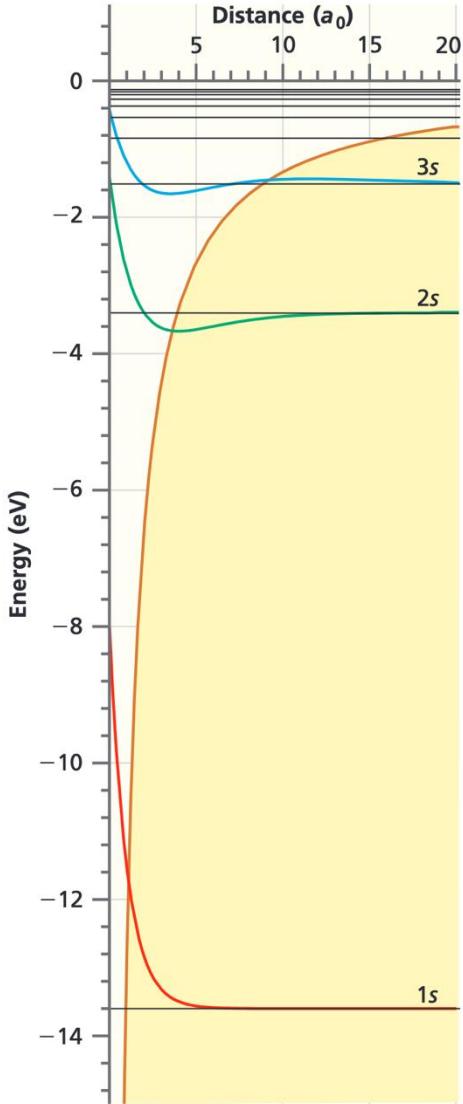
$$n = 2, l = 1 \quad R_{21}(r) = \frac{1}{\sqrt{24}} \left(\frac{1}{a_0} \right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}$$

$$n = 3, l = 0 \quad R_{30}(r) = \frac{2}{81\sqrt{3}} \left(\frac{1}{a_0} \right)^{3/2} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2} \right) e^{-r/3a_0}$$

$$n = 3, l = 1 \quad R_{31}(r) = \frac{4}{81\sqrt{6}} \left(\frac{1}{a_0} \right)^{3/2} \left(6\frac{r}{a_0} - \frac{r^2}{a_0^2} \right) e^{-r/3a_0}$$

$$n = 3, l = 2 \quad R_{32}(r) = \frac{4}{81\sqrt{30}} \left(\frac{1}{a_0} \right)^{3/2} \frac{r^2}{a_0^2} e^{-r/3a_0}$$

Egenverdier og ns -funksjoner



- Plott viser egenverdier og $R_{n0}(r)$
- Egenfunksjonene blir bredere og bredere
- Eksponentielt henfall i klassisk forbudt område (gul)
- Egenverdiene nærmer seg raskt null når n øker

Figure 9.2

Hydrogenorbitaler

Totale egenfunksjoner: H-orbitaler $\psi_{nlm} = R_{nl}(r)Y_l^m(\theta, \varphi)$

1s { $n = 1, l = 0, m_l = 0$ $\psi_{100}(r) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$

2s { $n = 2, l = 0, m_l = 0$ $\psi_{200}(r) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$

2p { $n = 2, l = 1, m_l = 0$ $\psi_{210}(r, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \cos \theta$

$n = 2, l = 1, m_l = \pm 1$ $\psi_{21\pm 1}(r, \theta, \phi) = \mp \frac{1}{8\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \sin \theta e^{\pm i\phi}$

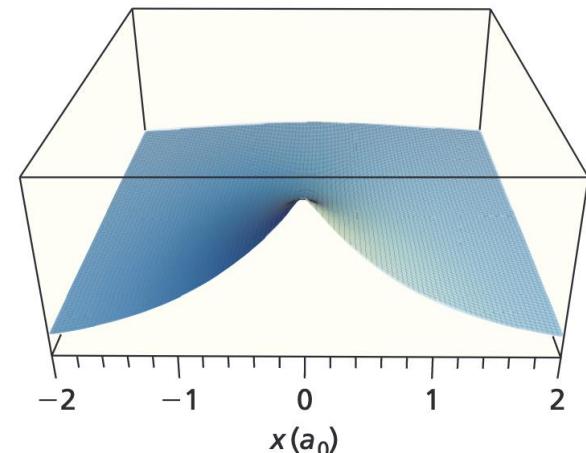
Generelt
komplekse
bølgefunktionsjoner ...

... fordi sfærisk
harmoniske er
komplekse ...

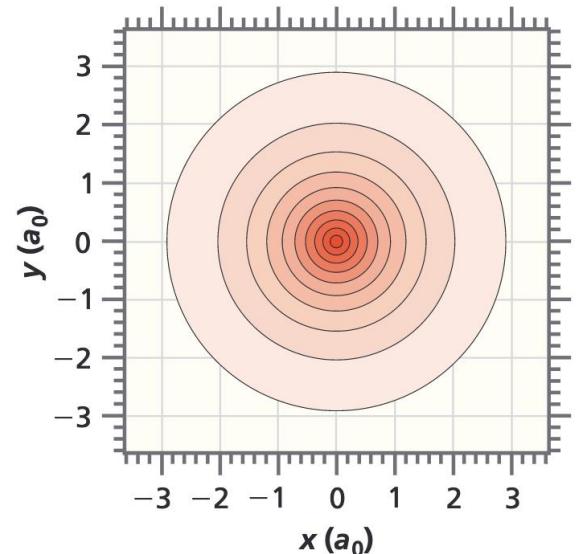
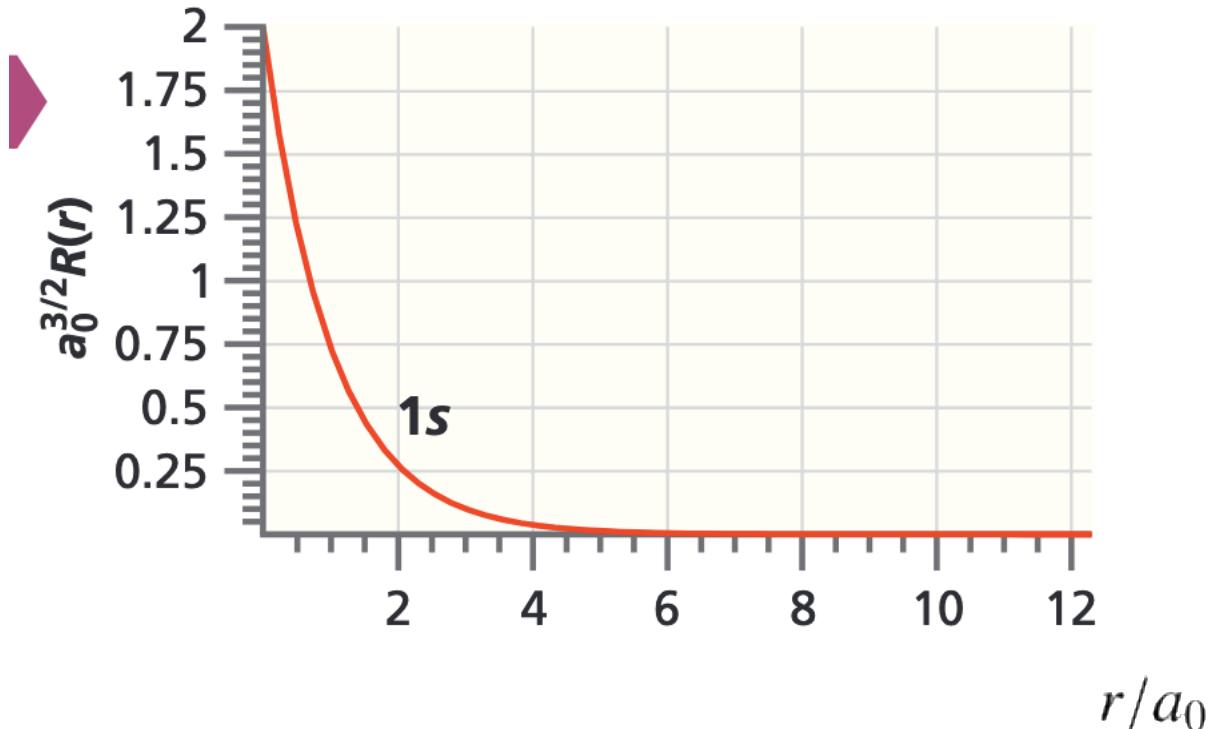
Visualisering

- Vi begynner forsiktig ...

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}$$



(a) 3D perspective



(b) Contour plot

Figure 9.4
Different images of $\psi_{100}(r)$. Diagrams are a (a) 3D perspective and (b) contour plot of $\psi_{100}(r)$. Darker contour colors indicate larger values for the magnitude of the amplitude.

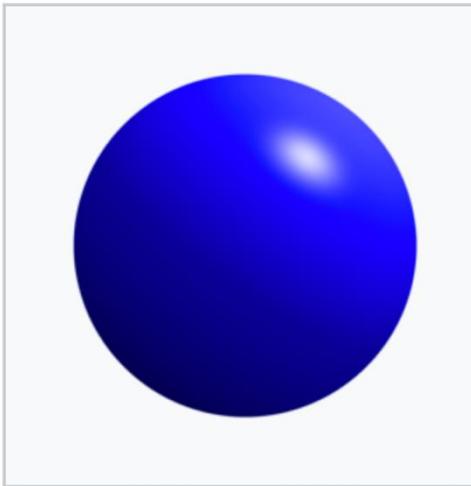
Isoflater

$$|\psi(r, \theta, \varphi)| = \text{konst.}$$

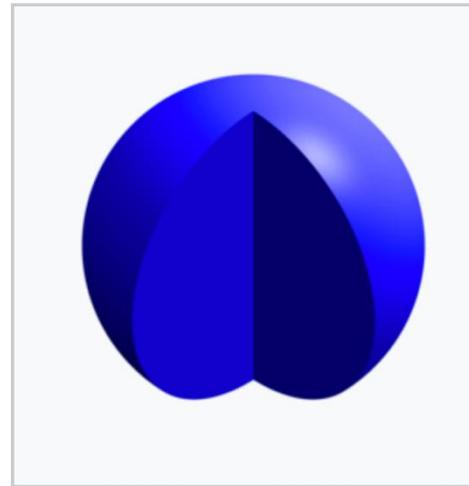
n = 1 [edit]

De punkter i rommet der funksjonen er konstant

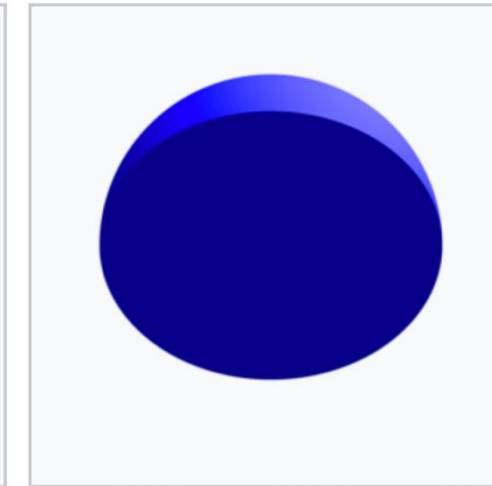
Vi skjærer vekk, kanskje er det struktur inni?



$n=1, l=0, m=0$

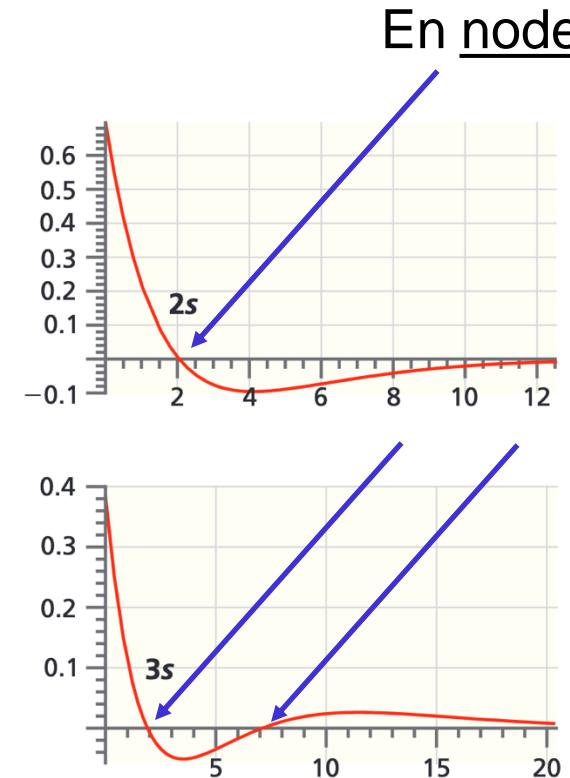
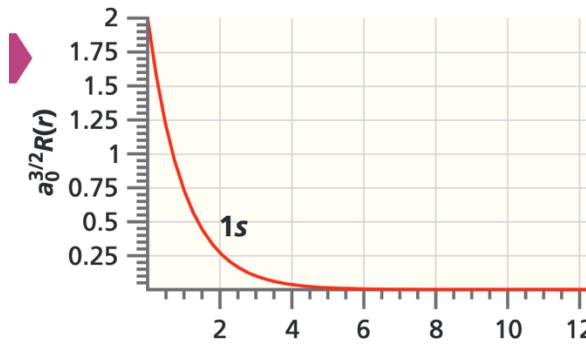


$n=1, l=0, m=0$



$n=1, l=0, m=0$

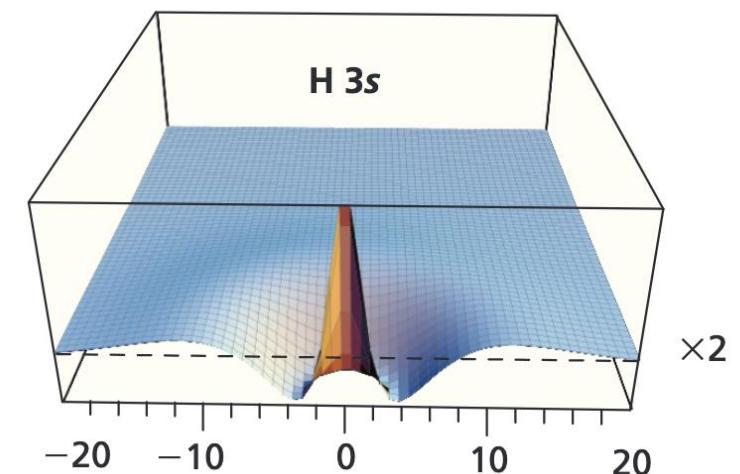
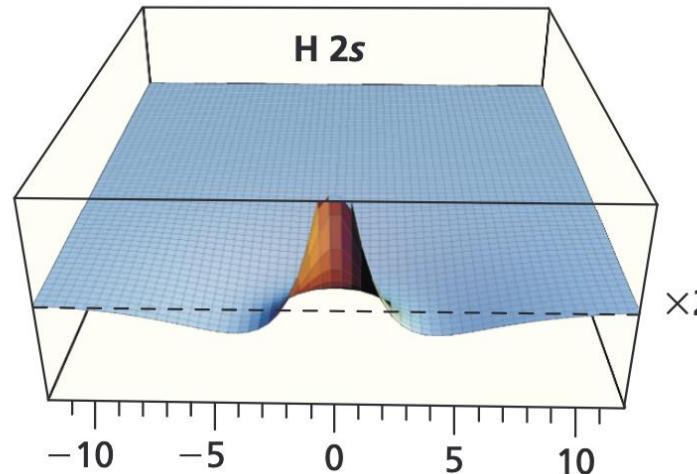
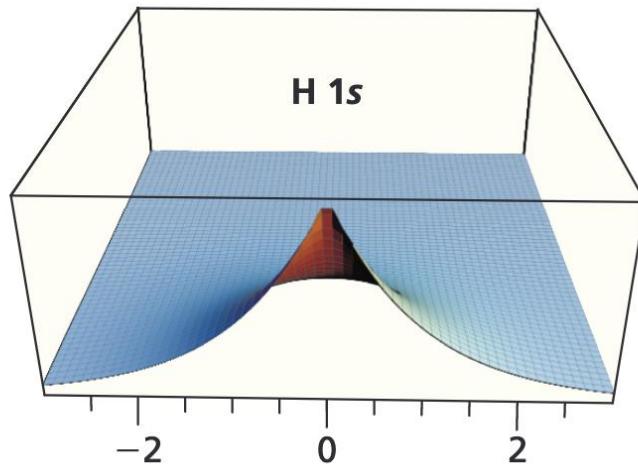
Flere radialfunksjoner



$$\#\text{noder} = n - l - 1$$

Bølgefunksjoner uten vinkelavhengighet

- Siden funksjonene er rotasjonssymmetriske kan vi visualisere ved å la feks $z=0$.

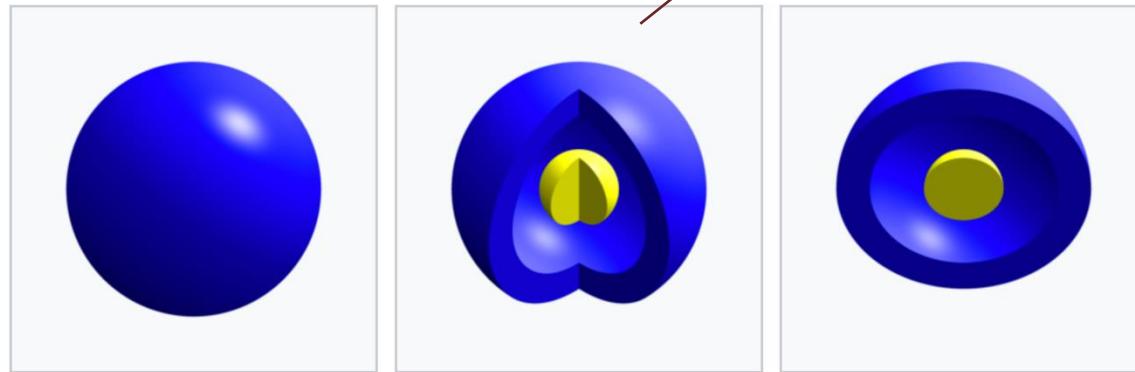


Isoflater for 2s og 3s

Vi skjærer vekk, kanskje
er det struktur inni?

$$|\psi(r, \theta, \varphi)| = \text{konst.}$$

n = 2 [edit]



n=2, l=0, m=0

n=2, l=0, m=0

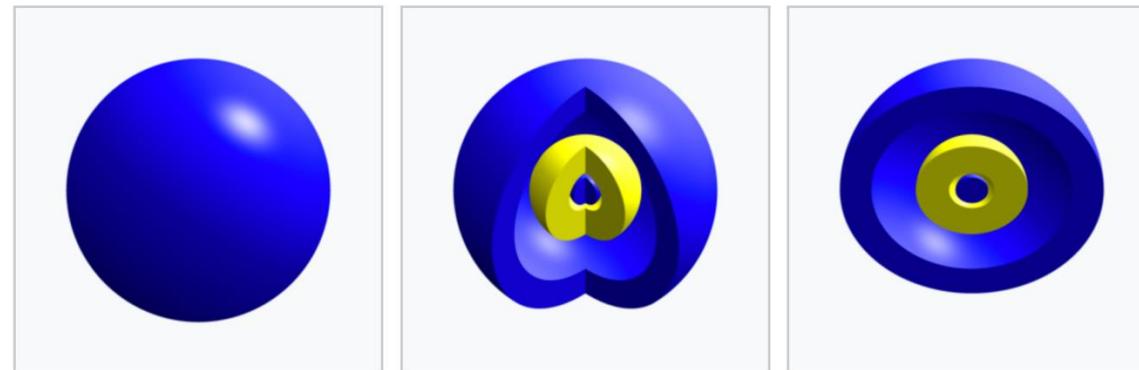
n=2, l=0, m=0

Blå = positiv verdi

Gul = negativ verdi

Hvor mange noder har 3s?

n = 3 [edit]



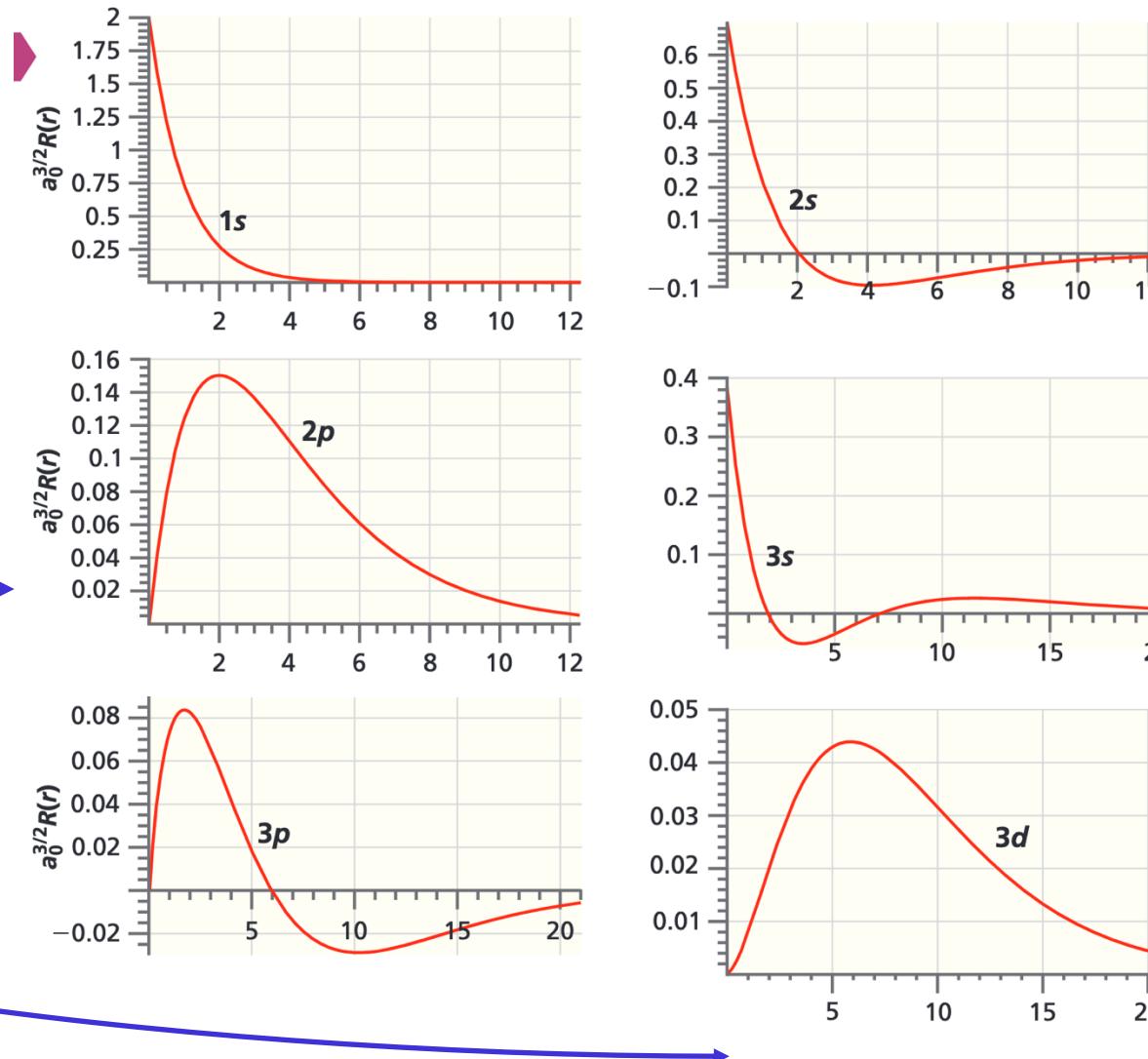
n=3, l=0, m=0

n=3, l=0, m=0

n=3, l=0, m=0

Flere radialfunksjoner

Men disse har
vinkelavhengighet ...



Relle sfærisk harmoniske

Reelle sfærisk harmoniske

- Sfærisk harmoniske er komplekse funksjoner:

$$Y_l^m(\theta, \phi) = N_{l,m} P_l^m(\cos \theta) e^{im\phi}$$

- Tar vi reell og imaginær del får vi lineært uavhengige egenfunksjoner for $\hat{\ell}^2$
- Vi tar en kikk på uttrykkene på neste slide ...

Fra komplekse til reelle sfærisk harmoniske

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

$\ell = 0$ [edit]

$$Y_{00} = \underline{s} = Y_0^0 = \frac{1}{2} \sqrt{\frac{1}{\pi}}$$

Merk notasjonen for s, p, d ... - funksjoner

$\ell = 1$ [edit]

$$Y_{1,-1} = \underline{p_y} = i \sqrt{\frac{1}{2}} (Y_1^{-1} + Y_1^1) = \sqrt{\frac{3}{4\pi}} \cdot \frac{y}{r} = \sqrt{\frac{3}{4\pi}} \sin(\theta) \sin \varphi$$

$$Y_{1,0} = \underline{p_z} = Y_1^0 = \sqrt{\frac{3}{4\pi}} \cdot \frac{z}{r} = \sqrt{\frac{3}{4\pi}} \cos(\theta)$$

$$Y_{1,1} = \underline{p_x} = \sqrt{\frac{1}{2}} (Y_1^{-1} - Y_1^1) = \sqrt{\frac{3}{4\pi}} \cdot \frac{x}{r} = \sqrt{\frac{3}{4\pi}} \sin(\theta) \cos \varphi$$

$\ell = 2$ [edit]

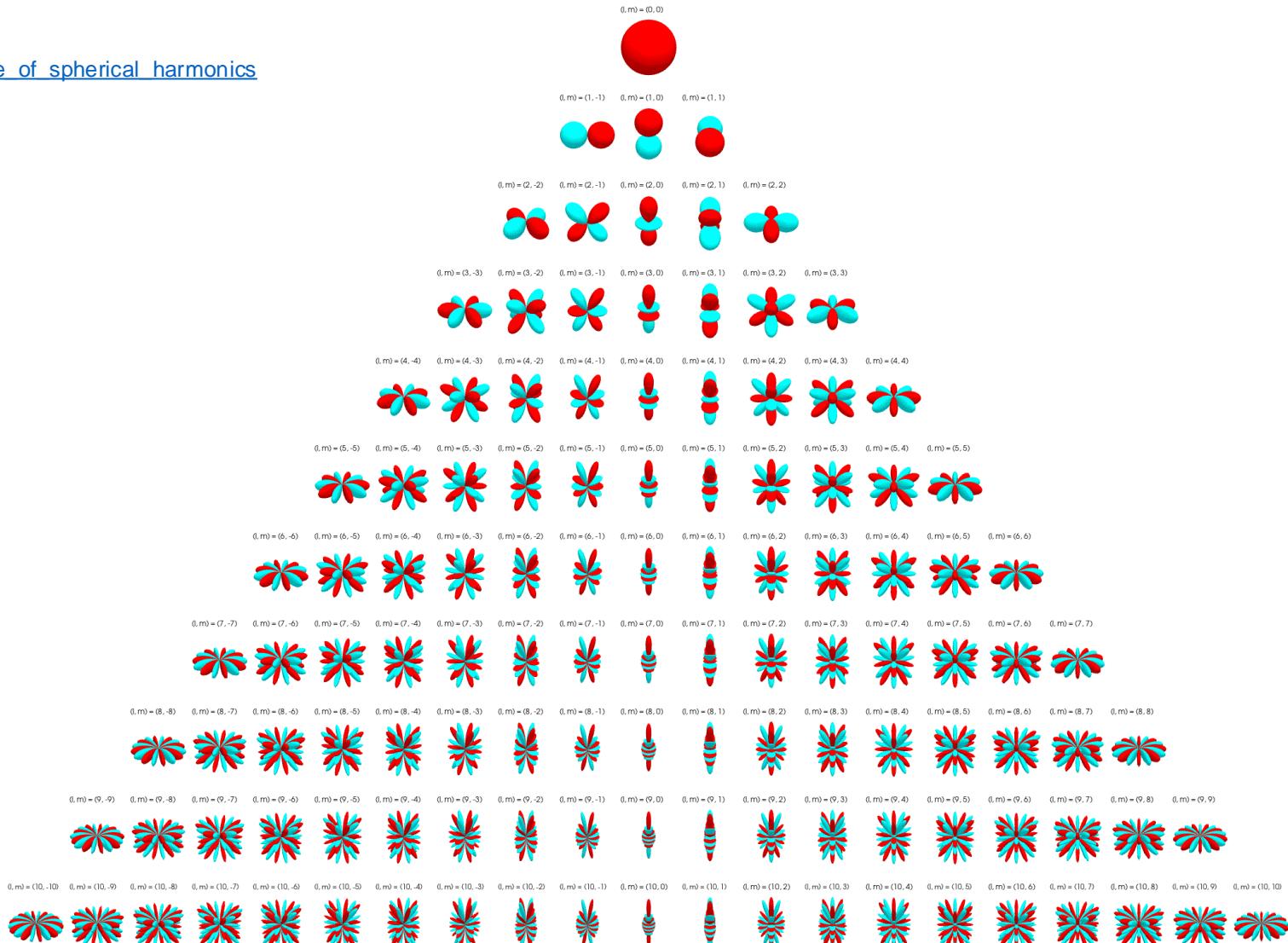
$$Y_{2,-2} = \underline{d_{xy}} = i \sqrt{\frac{1}{2}} (Y_2^{-2} - Y_2^2) = \frac{1}{2} \sqrt{\frac{15}{\pi}} \cdot \frac{xy}{r^2} = \frac{1}{4} \sqrt{\frac{15}{\pi}} \sin^2 \theta \sin(2\varphi)$$

$$Y_{2,-1} = \underline{d_{yz}} = i \sqrt{\frac{1}{2}} (Y_2^{-1} + Y_2^1) = \frac{1}{2} \sqrt{\frac{15}{\pi}} \cdot \frac{y \cdot z}{r^2} = \frac{1}{4} \sqrt{\frac{15}{\pi}} \sin(2\theta) \sin \varphi$$

Visualisering: standard polarplot

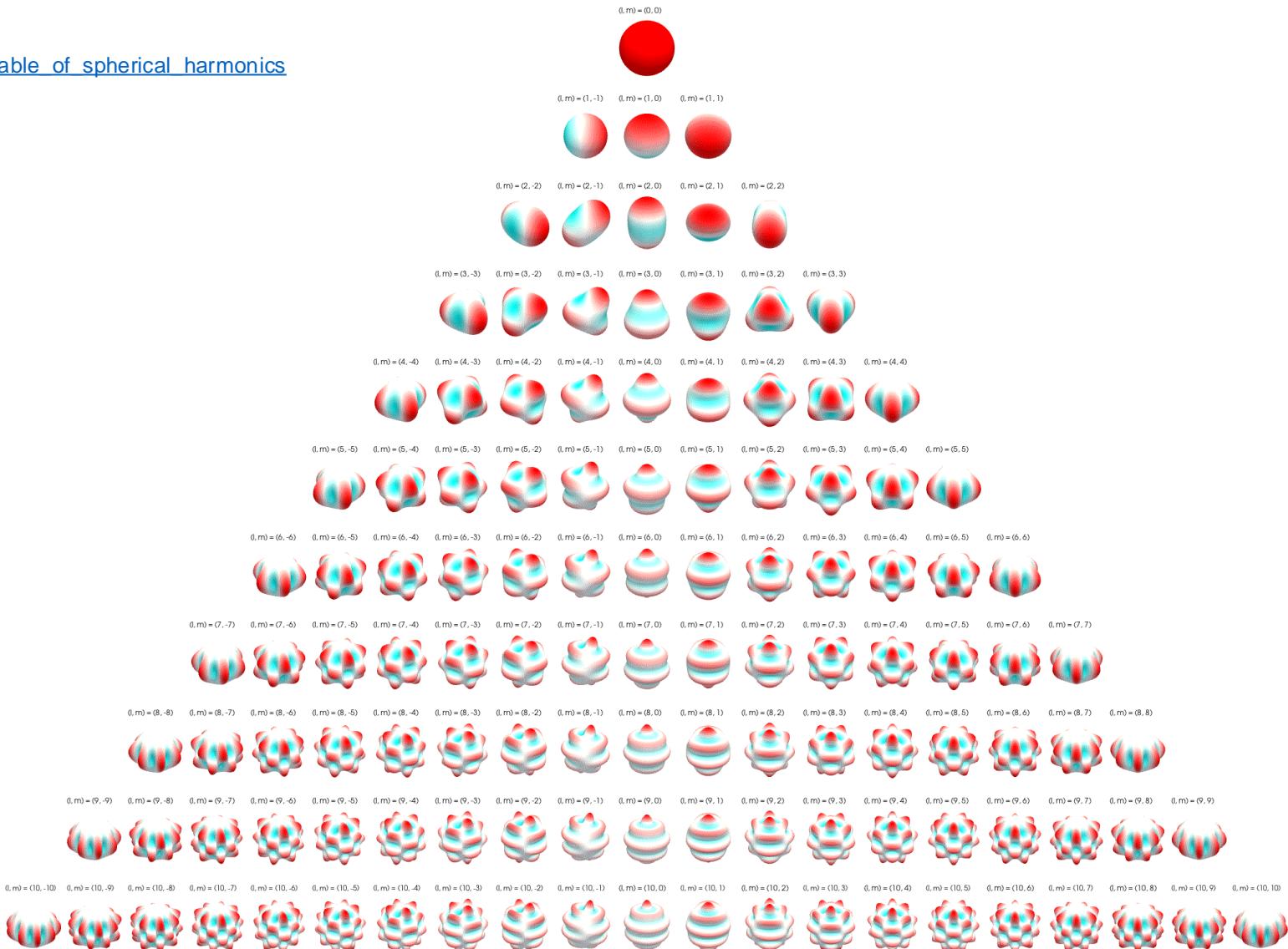
- https://en.wikipedia.org/wiki/Table_of_spherical_harmonics

- Klikk bildet



Visualisering: humpete plott

- https://en.wikipedia.org/wiki/Table_of_spherical_harmonics
- Klikk bildet



Reelle hydrogenorbitaler

Relle hydrogenorbitaler

$$\psi^{\text{reell}} = Y_{l,m}(\theta, \varphi)R_{n,l}(r)$$

m-index nede gir reelle
sfærisk harmoniske

Relle H-orbitaler, noen eksempler fra boka ...

$$\psi_{2p_x}(r, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \sin \theta \cos \phi$$

$$\psi_{2p_y}(r, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \sin \theta \sin \phi$$

$$\psi_{2p_z}(r, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \cos \theta$$

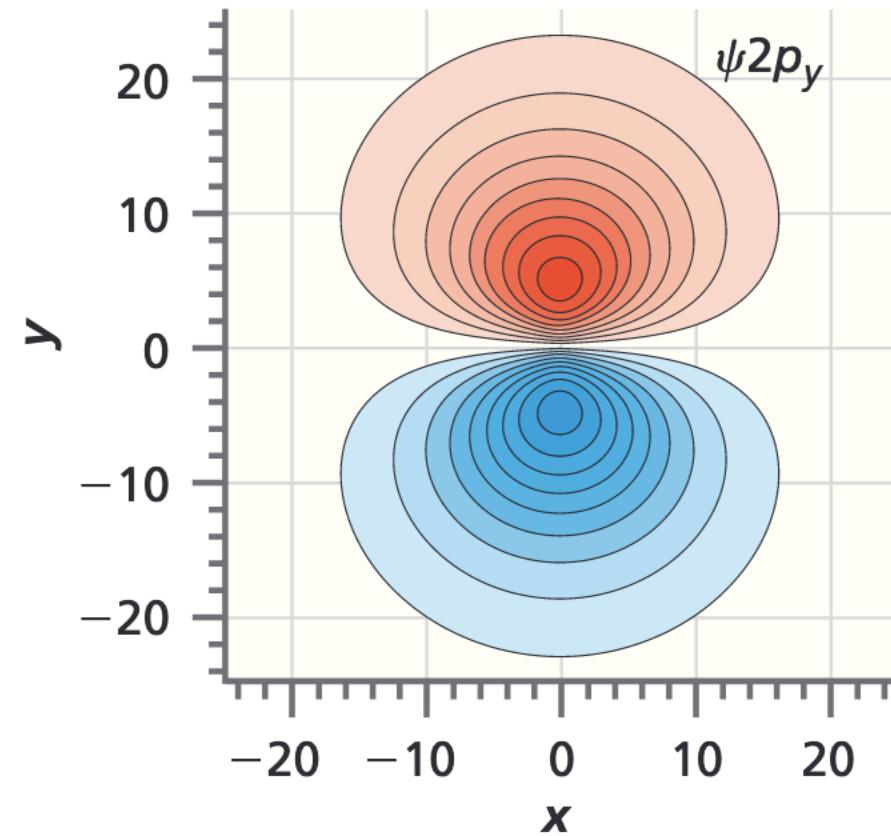
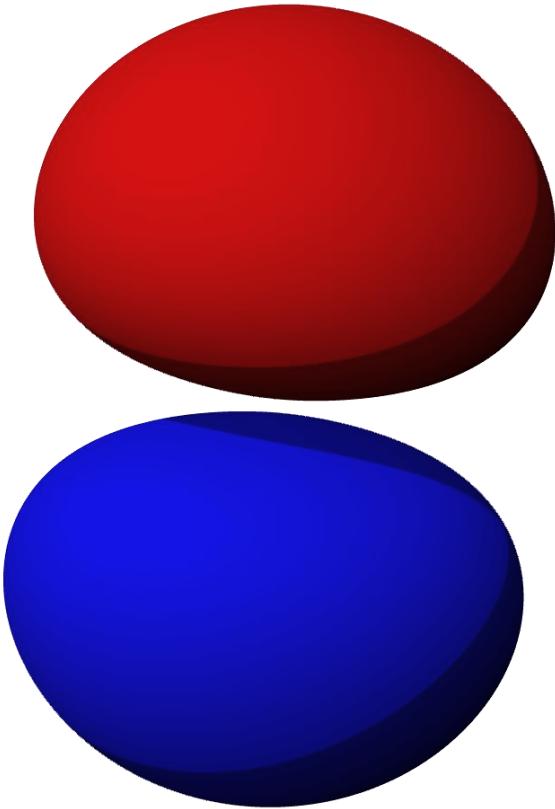
$$\psi_{3p_x}(r, \theta, \phi) = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(6\frac{r}{a_0} - \frac{r^2}{a_0^2}\right) e^{-r/3a_0} \sin \theta \cos \phi$$

$$\psi_{3p_y}(r, \theta, \phi) = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(6\frac{r}{a_0} - \frac{r^2}{a_0^2}\right) e^{-r/3a_0} \sin \theta \sin \phi$$

$$\psi_{3p_z}(r, \theta, \phi) = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} \left(6\frac{r}{a_0} - \frac{r^2}{a_0^2}\right) e^{-r/3a_0} \cos \theta$$

$$\psi_{3d_{z^2}}(r, \theta, \phi) = \frac{1}{81\sqrt{6\pi}} \left(\frac{1}{a_0}\right)^{3/2} \frac{r^2}{a_0^2} e^{-r/3a_0} (3 \cos^2 \theta - 1)$$

Isoflate vs. konturplott for $2p_y$



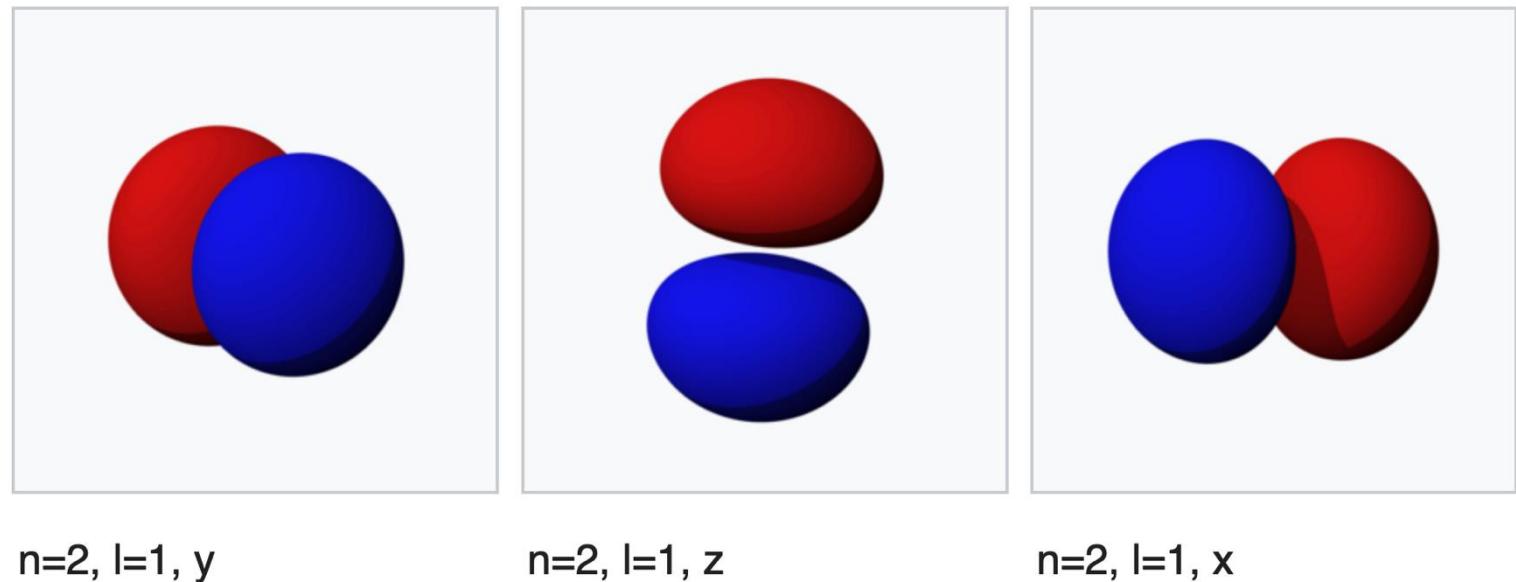
Isoflater for reelle H-orbitaler

- https://commons.wikimedia.org/wiki/Hydrogen_orbitals_3D_real
- 2p-funksjonene

$$2p_y = Y_{1,-1}(\theta, \varphi)R_{2,1}(r)$$

$$2p_z = Y_{1,0}(\theta, \varphi)R_{2,1}(r)$$

$$2p_x = Y_{1,1}(\theta, \varphi)R_{2,1}(r)$$



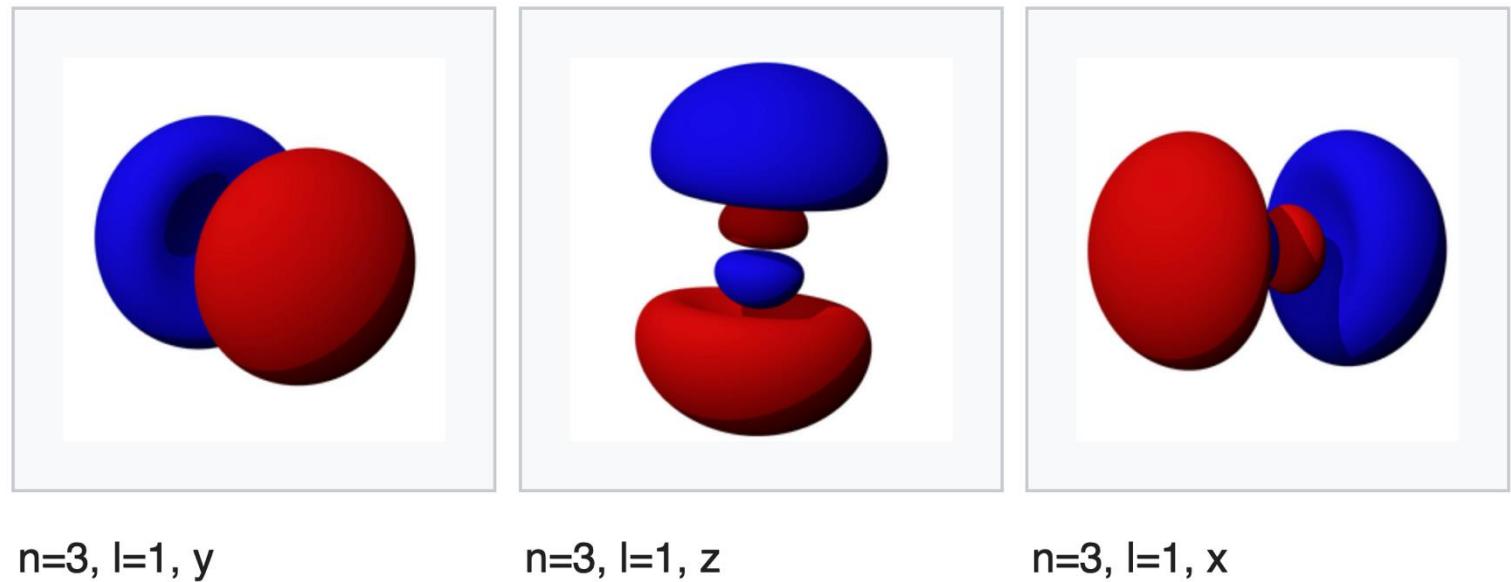
Isoflater for reelle H-orbitaler

- https://commons.wikimedia.org/wiki/Hydrogen_orbitals_3D_real
- 3p-funksjonene

$$3p_y = Y_{1,-1}(\theta, \varphi)R_{3,1}(r)$$

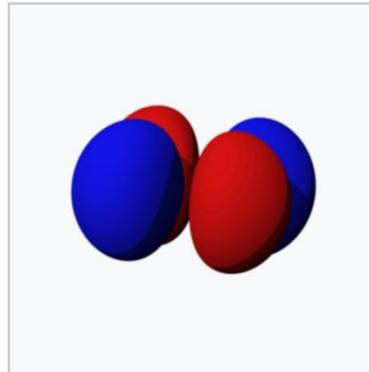
$$3p_z = Y_{1,0}(\theta, \varphi)R_{3,1}(r)$$

$$3p_x = Y_{1,1}(\theta, \varphi)R_{3,1}(r)$$

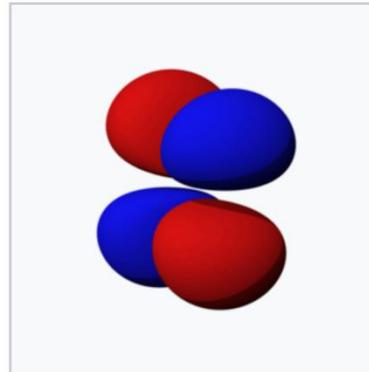


Isoflater for reelle H-orbitaler

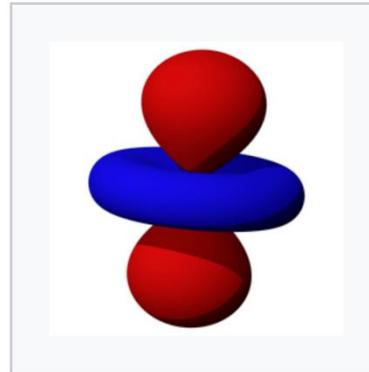
- https://commons.wikimedia.org/wiki/Hydrogen_orbitals_3D_real
- 3d-funksjonene



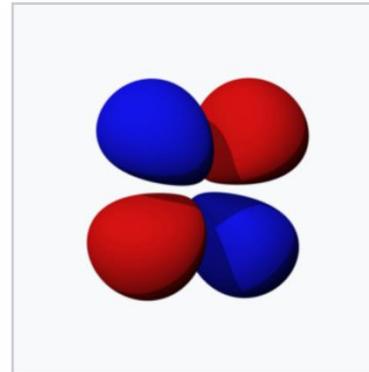
$n=3, l=2, x^2-y^2$



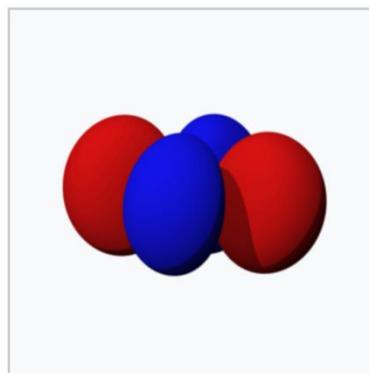
$n=3, l=2, yz$



$n=3, l=2, z^2$



$n=3, l=2, xz$



$n=3, l=2, xy$

Elektronskyer vs. isoflater

Visualisering som tetthet - positiv og negativ del har ulik farge

s p d

f

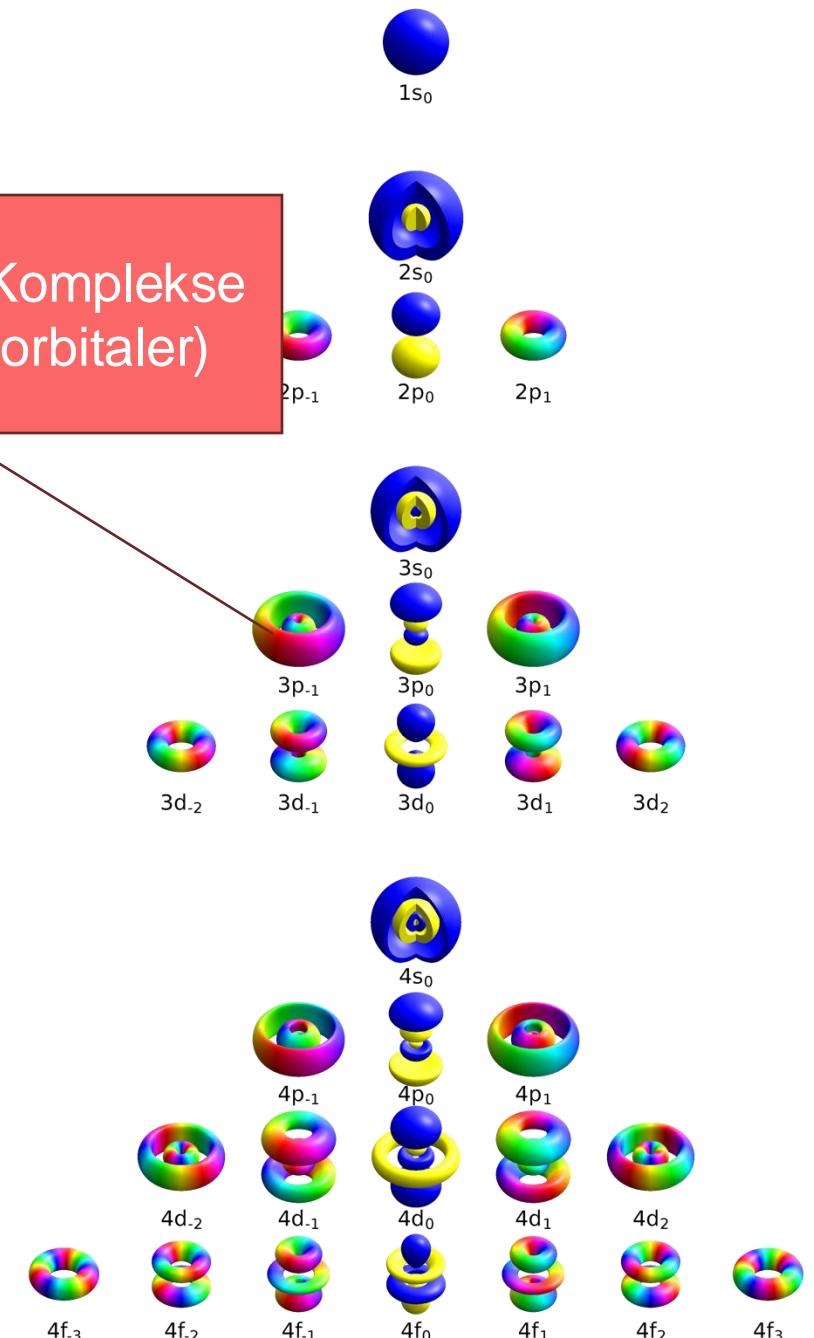
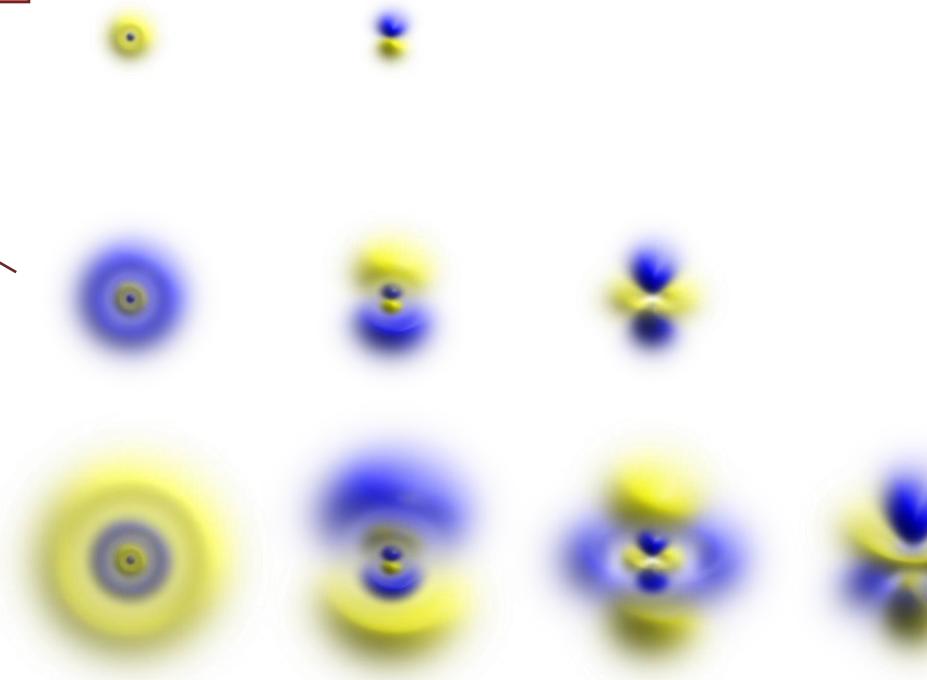
1

(Komplekse orbitaler)

2

3

4



Lenker til visualiseringer

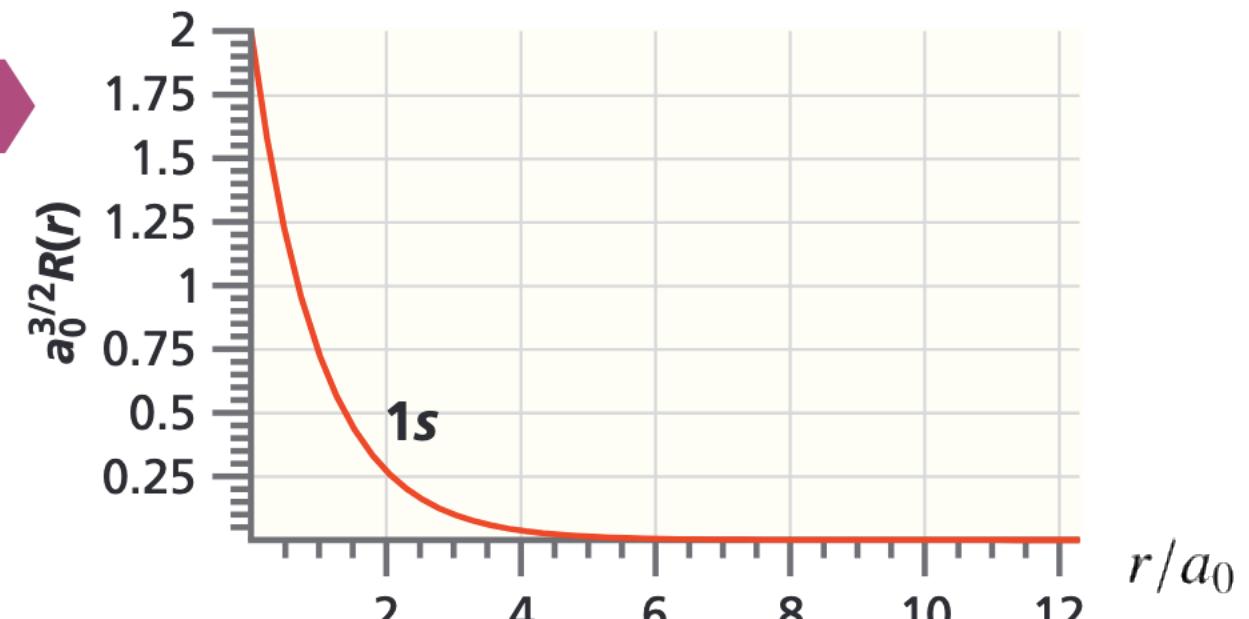
- https://commons.wikimedia.org/wiki/Hydrogen_orbitals_3D
- https://commons.wikimedia.org/wiki/Hydrogen_orbitals_3D_real
- https://commons.wikimedia.org/wiki/Category:Single_electron_orbitals
- [https://chem.libretexts.org/Courses/can/CHEM_210%3A_General_Chemistry_I_\(An_Atoms_Up_Approach\)/05%3A_The_Quantum_Model_of_the_Atom/5.07%3A_Atomic_Orbitals_and_Quantum_Numbers/5.7.01%3A_Visualizing_Atomic_Orbitals_as_Probability_Densities](https://chem.libretexts.org/Courses/can/CHEM_210%3A_General_Chemistry_I_(An_Atoms_Up_Approach)/05%3A_The_Quantum_Model_of_the_Atom/5.07%3A_Atomic_Orbitals_and_Quantum_Numbers/5.7.01%3A_Visualizing_Atomic_Orbitals_as_Probability_Densities)
- <https://www.chm.davidson.edu/vce/AtomicOrbitals/AtomicOrbitals-Visualization.html>
- <https://winter.group.shef.ac.uk/orbitron/>

Sannsynlighetstolkning

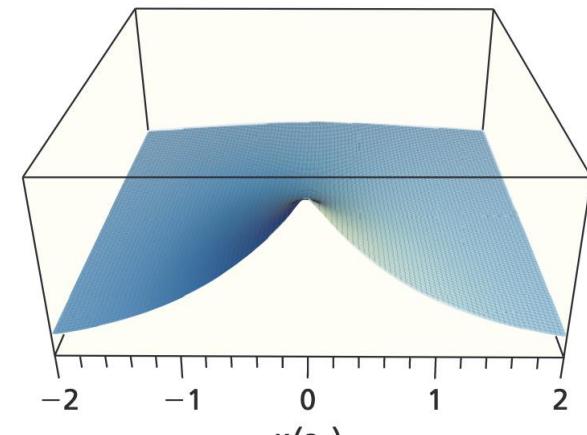
1s-orbitalen

- Hvor er elektronet mest sannsynligvis?

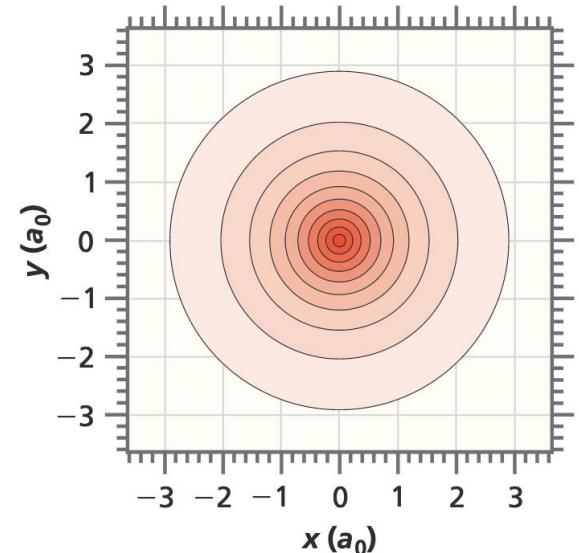
$$\psi_{100}(r) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}$$



$$P(\mathbf{r}) = \frac{1}{\pi a_0^3} e^{-2r/a_0}$$



(a) 3D perspective



(b) Contour plot

Figure 9.4

Different images of $\psi_{100}(r)$. Diagrams are a (a) 3D perspective and (b) contour plot of $\psi_{100}(r)$. Darker contour colors indicate larger values for the magnitude of the amplitude.

Størst sannsynlighet nær kjernen ...

- Virker urimelig – var ikke problemet i klassisk fysikk at elektronet ville kollapse inn i kjernen?
- Jo, men sannsynligheten for å finne elektronet «inne i» kjernen er forsvinnende liten, se Example Problem 9.4:

$$P = \frac{1}{6} \left(\frac{r_{nucleus}}{a_0} \right)^3 = 9.0 \times 10^{-15}$$

Hva er sannsynligheten for å finne elektronet i en avstand r fra kjernen?

- Må integrere opp sannsynligheten over et kuleskall med radius r

$$P_{nl}(r) dr = \left[\int_0^{2\pi} d\phi \int_0^{\pi} (Y_l^{m_l}(\theta, \phi))^* (Y_l^{m_l}(\theta, \phi)) \sin \theta d\theta \right] r^2 R_{nl}^2(r) dr = r^2 R_{nl}^2(r) dr \quad (9.13)$$

IKKE sannsynlighet for posisjon –
men avstand!

Radialdistribusjoner

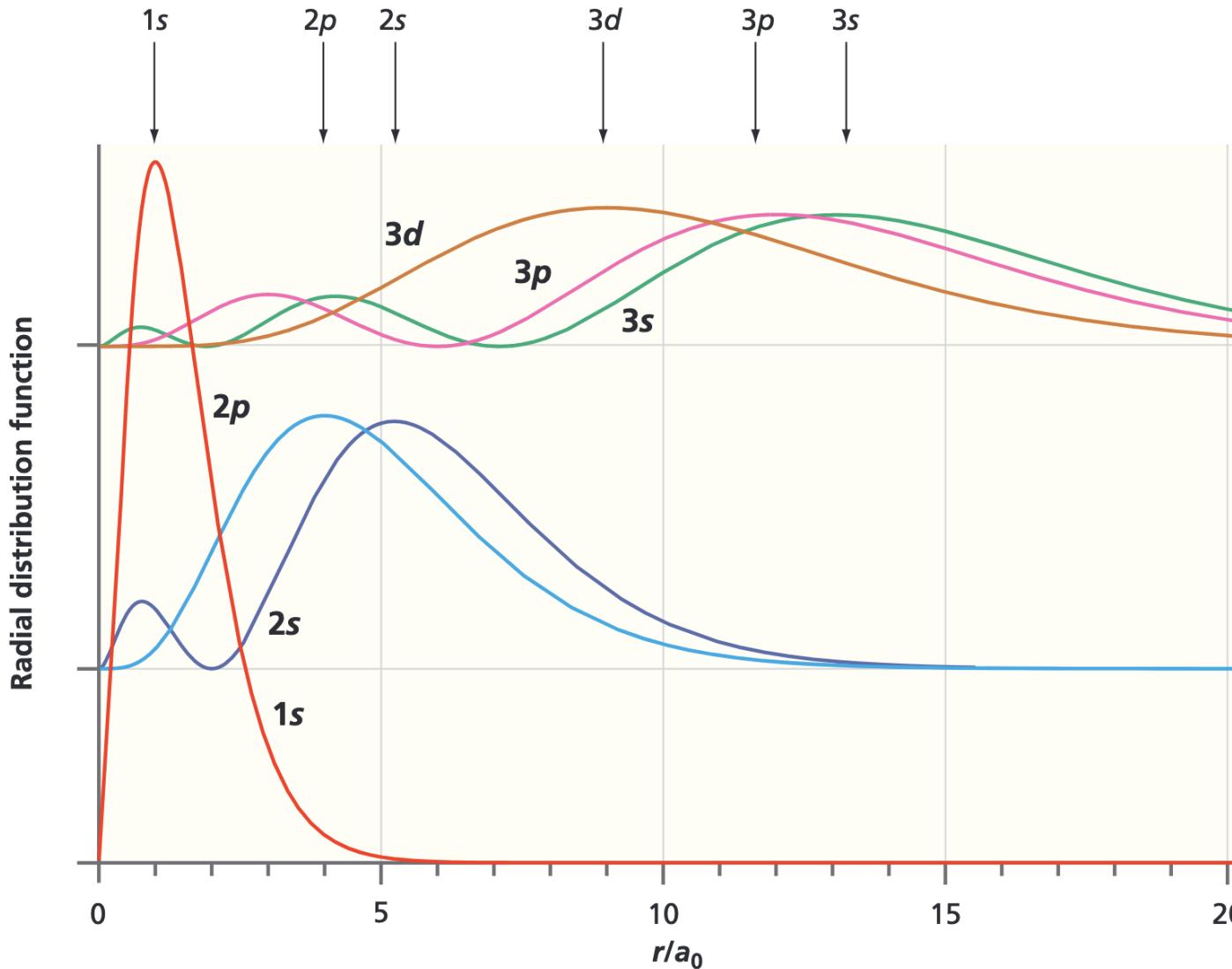


Figure 9.10
Plot of $r^2 R_{nl}^2(r)$ versus r/a_0 for the first few H atomic orbitals. The curves for $n = 2$ and $n = 3$ have been displaced vertically as indicated. The position of the principal maximum for each orbital is indicated by an arrow.

Skallmodellen – kan vi se Bohrs modell i radialfordelingen?

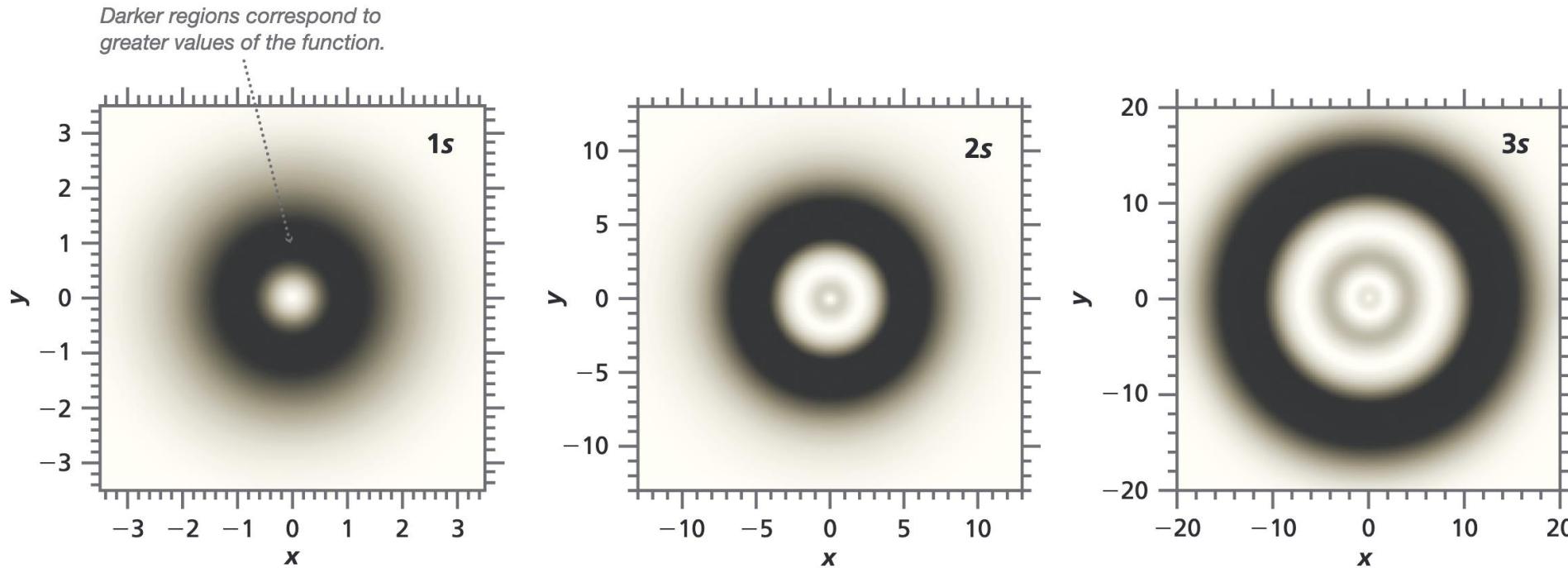


Figure 9.12

The radial probability distribution evaluated for $z = 0$ for the 1s, 2s, and 3s orbitals. The view is in the $x - y$ plane and lengths are in units of a_0 . Darker regions correspond to greater values of the function. The sharp circle in a classical shell model becomes a broad ring in a quantum-mechanical model over which the probability of finding the electron varies. Less intense subsidiary rings are also observed for the 2s and 3s orbitals.