

# Väteatomen

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Löstes av Schrödinger 1926.  
Visar att Schrödingerekvationen fungerar!

$$SE \text{ i } 3D: -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + V(\vec{r}) \Psi(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t)$$

Sannolikhetsfökninng:

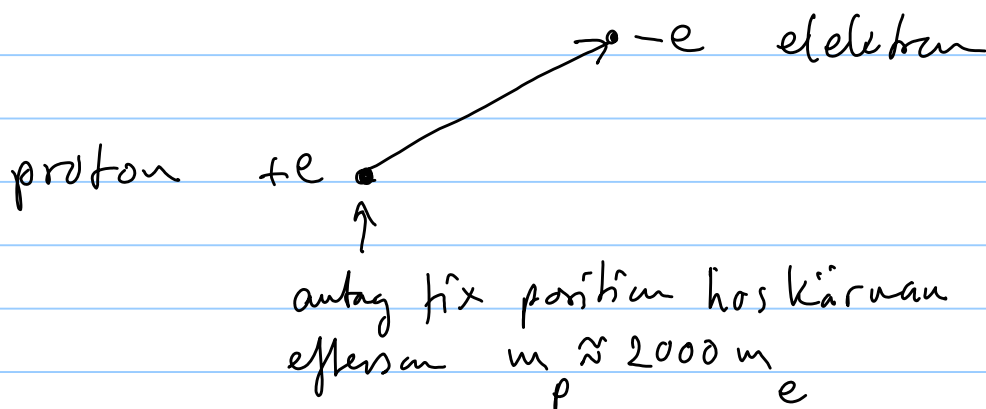
$|\Psi(\vec{r}, t)|^2 d^3r$  = sannolikhet att hitta partikeln i volymelementet  $d^3r$  i  $\vec{r}$  vid tiden  $t$ .

Normering:  $\int |\Psi(\vec{r}, t)|^2 d^3r = 1$

Stationära tillstånd:  $\Psi(\vec{r}, t) = \psi(\vec{r}) e^{-iEt/\hbar}$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$$

## Väteatomen



$$V(\vec{r}) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \quad \text{Coulomb potential}$$

$$\frac{1}{4\pi\epsilon_0} \approx 9 \cdot 10^9 \text{ Nm}^2 \text{ C}^{-2}$$

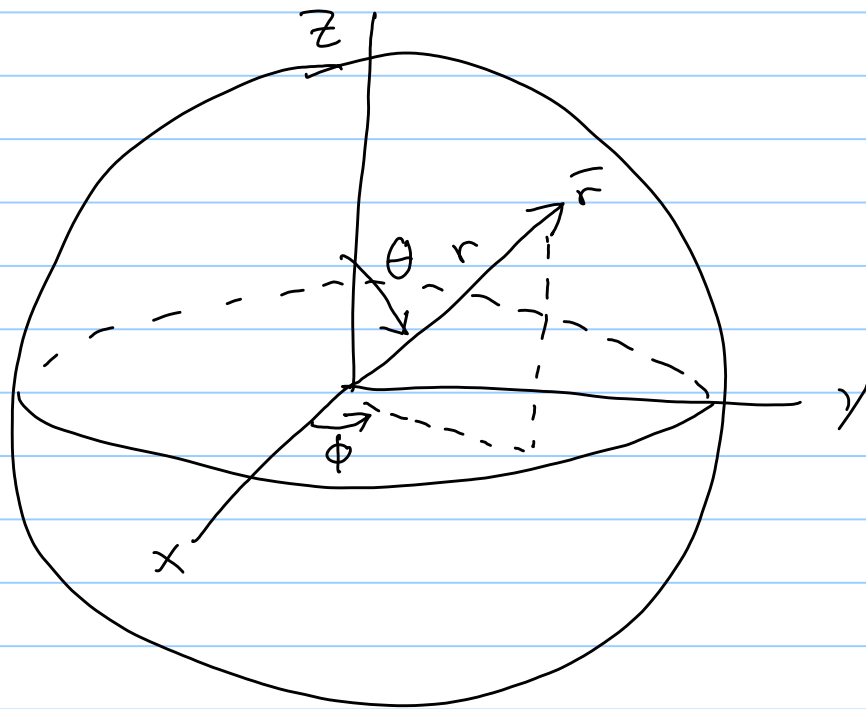
Table with the del operator in cylindrical and spherical coordinates

Operation	Cartesian coordinates (x,y,z)	Cylindrical coordinates (ρ,φ,z)	Spherical coordinates (r,θ,φ)
Definition of coordinates	$\rho = \sqrt{x^2 + y^2}$ $\phi = \arctan(y/x)$ $z = z$	$x = \rho \cos \phi$ $y = \rho \sin \phi$ $z = z$	$x = r \sin \theta \cos \phi$ $y = r \sin \theta \sin \phi$ $z = r \cos \theta$
	$r = \sqrt{x^2 + y^2 + z^2}$ $\theta = \arctan\left(\frac{\sqrt{x^2 + y^2}}{z}\right)$ $\phi = \arctan(y/x)$	$r = \sqrt{\rho^2 + z^2}$ $\theta = \arctan(\rho/z)$ $\phi = \phi$	$\rho = r \sin(\theta)$ $\phi = \phi$ $z = r \cos(\theta)$
Definition of unit vectors	$\hat{\rho} = \frac{x}{\rho}\hat{x} + \frac{y}{\rho}\hat{y}$ $\hat{\phi} = -\frac{y}{\rho}\hat{x} + \frac{x}{\rho}\hat{y}$ $\hat{z} = \hat{z}$	$\hat{x} = \cos \phi \hat{\rho} - \sin \phi \hat{\phi}$ $\hat{y} = \sin \phi \hat{\rho} + \cos \phi \hat{\phi}$ $\hat{z} = \hat{z}$	$\hat{x} = \sin \theta \cos \phi \hat{r} + \cos \theta \cos \phi \hat{\theta} - \sin \phi \hat{\phi}$ $\hat{y} = \sin \theta \sin \phi \hat{r} + \cos \theta \sin \phi \hat{\theta} + \cos \phi \hat{\phi}$ $\hat{z} = \cos \theta \hat{r} - \sin \theta \hat{\theta}$
	$\hat{r} = \frac{x\hat{x} + y\hat{y} + z\hat{z}}{r}$ $\hat{\theta} = \frac{zx\hat{x} + yz\hat{y} - \rho^2\hat{z}}{r\rho}$ $\hat{\phi} = \frac{-y\hat{x} + x\hat{y}}{\rho}$	$\hat{r} = \frac{\rho}{r}\hat{\rho} + \frac{z}{r}\hat{z}$ $\hat{\theta} = \frac{z}{r}\hat{\rho} - \frac{\rho}{r}\hat{z}$ $\hat{\phi} = \hat{\phi}$	$\hat{\rho} = \sin \theta \hat{r} + \cos \theta \hat{\theta}$ $\hat{\phi} = \hat{\phi}$ $\hat{z} = \cos \theta \hat{r} - \sin \theta \hat{\theta}$
A vector field <b>A</b>	$A_x\hat{x} + A_y\hat{y} + A_z\hat{z}$	$A_\rho\hat{\rho} + A_\phi\hat{\phi} + A_z\hat{z}$	$A_r\hat{r} + A_\theta\hat{\theta} + A_\phi\hat{\phi}$
Gradient $\nabla f$	$\frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial z}\hat{z}$	$\frac{\partial f}{\partial \rho}\hat{\rho} + \frac{1}{\rho}\frac{\partial f}{\partial \phi}\hat{\phi} + \frac{\partial f}{\partial z}\hat{z}$	$\frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r \sin \theta}\frac{\partial f}{\partial \phi}\hat{\phi}$
Divergence $\nabla \cdot \mathbf{A}$	$\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z}$	$\frac{1}{\rho}\frac{\partial(\rho A_\rho)}{\partial \rho} + \frac{1}{\rho}\frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z}$	$\frac{1}{r^2}\frac{\partial(r^2 A_r)}{\partial r} + \frac{1}{r \sin \theta}\frac{\partial}{\partial \theta}(A_\theta \sin \theta) + \frac{1}{r \sin \theta}\frac{\partial A_\phi}{\partial \phi}$
Curl $\nabla \times \mathbf{A}$	$\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\hat{x} + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\hat{y} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{z}$	$\left(\frac{1}{\rho}\frac{\partial A_z}{\partial \phi} - \frac{\partial A_\phi}{\partial z}\right)\hat{\rho} + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial \rho}\right)\hat{\phi} + \frac{1}{\rho}\left(\frac{\partial(\rho A_\phi)}{\partial \rho} - \frac{\partial A_\rho}{\partial \phi}\right)\hat{z}$	$\frac{1}{r \sin \theta}\left(\frac{\partial}{\partial \theta}(A_\phi \sin \theta) - \frac{\partial A_\theta}{\partial \phi}\right)\hat{r} + \frac{1}{r}\left(\frac{1}{\sin \theta}\frac{\partial A_r}{\partial \phi} - \frac{\partial}{\partial r}(r A_\phi)\right)\hat{\theta} + \frac{1}{r}\left(\frac{\partial}{\partial r}(r A_\theta) - \frac{\partial A_r}{\partial \theta}\right)\hat{\phi}$
Laplace operator $\Delta f = \nabla^2 f$	$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$	$\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial f}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2}$	$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin \theta}\frac{\partial}{\partial \theta}\left(\sin \theta\frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2 \theta}\frac{\partial^2 f}{\partial \phi^2}$
Vector Laplacian $\Delta \mathbf{A} = \nabla^2 \mathbf{A}$	$\Delta A_x\hat{x} + \Delta A_y\hat{y} + \Delta A_z\hat{z}$	$\left(\Delta A_\rho - \frac{A_\rho}{\rho^2} - \frac{2}{\rho^2}\frac{\partial A_\phi}{\partial \phi}\right)\hat{\rho} + \left(\Delta A_\phi - \frac{A_\phi}{\rho^2} + \frac{2}{\rho^2}\frac{\partial A_\rho}{\partial \phi}\right)\hat{\phi} + (\Delta A_z)\hat{z}$	$\left(\Delta A_r - \frac{2A_r}{r^2} - \frac{2}{r^2 \sin \theta}\frac{\partial(A_\theta \sin \theta)}{\partial \theta} - \frac{2}{r^2 \sin \theta}\frac{\partial A_\phi}{\partial \phi}\right)\hat{r} + \left(\Delta A_\theta - \frac{A_\theta}{r^2 \sin^2 \theta} + \frac{2}{r^2}\frac{\partial A_r}{\partial \theta} - \frac{2 \cos \theta}{r^2 \sin^2 \theta}\frac{\partial A_\phi}{\partial \phi}\right)\hat{\theta} + \left(\Delta A_\phi - \frac{A_\phi}{r^2 \sin^2 \theta} + \frac{2}{r^2 \sin \theta}\frac{\partial A_r}{\partial \phi} + \frac{2 \cos \theta}{r^2 \sin^2 \theta}\frac{\partial A_\theta}{\partial \phi}\right)\hat{\phi}$
Differential displacement	$d\mathbf{l} = dx\hat{x} + dy\hat{y} + dz\hat{z}$	$d\mathbf{l} = d\rho\hat{\rho} + \rho d\phi\hat{\phi} + dz\hat{z}$	$d\mathbf{l} = dr\hat{r} + r d\theta\hat{\theta} + r \sin \theta d\phi\hat{\phi}$
Differential normal area	$d\mathbf{S} = dy dz \hat{x} + dx dz \hat{y} + dx dy \hat{z}$	$d\mathbf{S} = \rho d\phi dz \hat{\rho} + d\rho dz \hat{\phi} + \rho d\rho d\phi \hat{z}$	$d\mathbf{S} = r^2 \sin \theta d\theta d\phi \hat{r} + r \sin \theta dr d\phi \hat{\theta} + r dr d\theta \hat{\phi}$
Differential volume	$dv = dx dy dz$	$dv = \rho d\rho d\phi dz$	$dv = r^2 \sin \theta dr d\theta d\phi$

Non-trivial calculation rules:

1.  $\text{div grad } f = \nabla \cdot (\nabla f) = \nabla^2 f = \Delta f$  (Laplacian)
2.  $\text{curl grad } f = \nabla \times (\nabla f) = \mathbf{0}$
3.  $\text{div curl } \mathbf{A} = \nabla \cdot (\nabla \times \mathbf{A}) = \mathbf{0}$
4.  $\text{curl curl } \mathbf{A} = \nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$  (using Lagrange's formula for the cross product)
5.  $\Delta fg = f\Delta g + 2\nabla f \cdot \nabla g + g\Delta f$

# Sfäriska koordinater



$$\vec{r} = r (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$$

$$\left\{ \begin{array}{l} r = \sqrt{x^2 + y^2 + z^2} \end{array} \right.$$

$$\left\{ \begin{array}{l} \theta = \arccos \frac{z}{r} \quad (\text{polär vinkel el. zenit, colatitud}) \end{array} \right.$$

$$\left\{ \begin{array}{l} \phi = \arctan \frac{y}{x} \quad (\text{azimuthvinkel el. longitud}) \end{array} \right.$$

$$\Delta \psi: \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) +$$

$$+ \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$= \frac{e^2}{4\pi \epsilon_0 r} + E$$

Variablen Separation:  $\Psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$

$$\Rightarrow \frac{\sin^2 \theta}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} + \frac{2m r^2 \sin^2 \theta}{\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) = 0$$

wähle von konstant =  $-m_l^2$

$$\Rightarrow \frac{1}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{2m r^2}{\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) = \frac{m_l^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right)$$

wähle von konstant =  $l(l+1)$

Ges 3 ordn. d.e.

$$\left\{ \begin{array}{l} \frac{d^2 \Phi}{d\phi^2} + m_l^2 \Phi = 0 \\ \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \left[ l(l+1) - \frac{m_l^2}{\sin^2 \theta} \right] \Theta = 0 \\ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left[ \frac{2m}{\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E \right) - \frac{l(l+1)}{r^2} \right] R = 0 \end{array} \right.$$

Fullständig lösning av dessa ekvationer  
Andras i kommande kurer i kvantmekanik.  
Vi ska här bara göra de enklaste stegen,  
och i ömångt ge resultaten utan härledning.

Lösning i  $\phi$ -led:

$$\frac{d^2 \Phi}{d\phi^2} + m_l^2 \Phi = 0 \Rightarrow \Phi(\phi) = e^{i m_l \phi}$$

$\phi$  är  $2\pi$ -periodisk:  $\Phi(\phi + 2\pi) = \Phi(\phi) \Rightarrow$   
 $e^{i m_l (\phi + 2\pi)} = e^{i m_l \phi} \Rightarrow e^{i 2\pi m_l} = 1$

$\Rightarrow m_l = 0, \pm 1, \pm 2, \dots, \pm l$

Kan visa: maximala  $|m_l|$  är  $= l$

$m_l$  kallas magnetiska kvanttalet

Kan visa: Energivärdena ges av

$$E_n = - \frac{m e^4}{32 \pi^2 \epsilon_0^2 \hbar^2} \frac{1}{n^2} = - \frac{13.6 \text{ eV}}{n^2}$$

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

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

# Balkvantisering

vill försöka tolka denna term

Radiella ekvationen:

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \left[ \frac{2m}{\hbar^2} \left( \frac{e^2}{4\pi\epsilon_0 r} + E - \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] R = 0$$

tolka detta som  $= E_{\text{radial}} + E_{\text{kin}}$

eftersom det gäller (klamret):  $E = E_{\text{kin}}^{\text{radial}} + E_{\text{kin}}^{\text{ban}} - \frac{e^2}{4\pi\epsilon_0 r}$

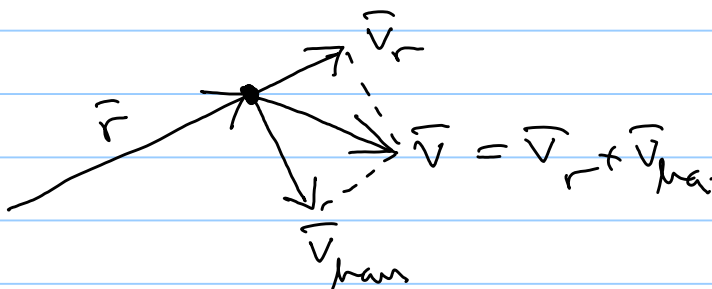
För att den radiella ekvationen även endast ska bero på  $E_{\text{kin}}^{\text{radial}}$  antar vi nu att de två extra energitermen tar ut varandra

$$\therefore E_{\text{kin}}^{\text{ban}} = \frac{\hbar^2 l(l+1)}{2mr^2}$$

Vi argumenterar nu för att  $E_{\text{kin}}^{\text{ban}} = \frac{L^2}{2mr^2}$

där  $\vec{L} = \vec{r} \times \vec{p}$  är rörelsemängdsmomentet:

$$\vec{L} = \vec{r} \times \vec{p} = m \vec{r} \times \vec{v} \Rightarrow L = m r v_{\text{ban}}$$


$$\Rightarrow E_{\text{kin}}^{\text{ban}} = \frac{1}{2} m v_{\text{ban}}^2 = \frac{L^2}{2mr^2}$$

Alltså är rörelsemängdsmomentet

$$L^2 = l(l+1) \hbar^2, \quad L = \sqrt{l(l+1)} \hbar$$

Z-komponenten:  $L_z = m_l \hbar$ ,  $m_l = 0, \pm 1, \dots, \pm l$

## Egenfunktioner till rörelsemängdsmomentet

$$\hat{L}^2 Y_l^m = l(l+1)\hbar^2 Y_l^m, \quad l=0, 1, 2, \dots$$

$$\hat{L}_z Y_l^m = m\hbar Y_l^m, \quad m=-l, \dots, l-1, l$$

$$\int Y_{l'}^{m'} Y_l^m d\Omega = \delta_{l'l} \delta_{m'm}$$

$$d\Omega = \sin\theta d\theta d\phi$$

## Klotfunktioner (spherical harmonics)

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

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

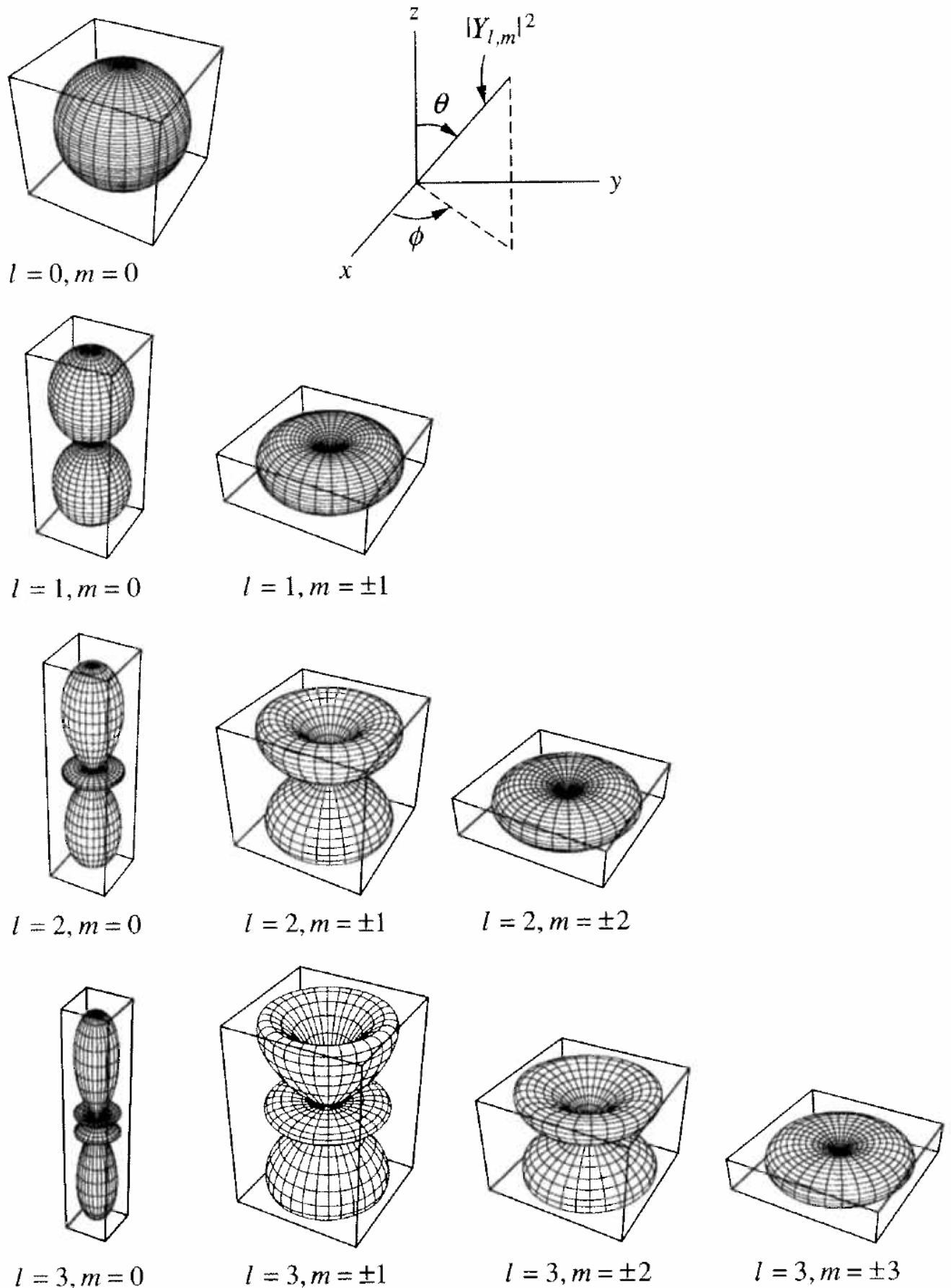
$$Y_1^{\pm 1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi} = \mp \sqrt{\frac{3}{8\pi}} \frac{x \pm iy}{r}$$

$$Y_2^0 = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1) = \sqrt{\frac{5}{16\pi}} \frac{3z^2 - r^2}{r^2}$$

$$Y_2^{\pm 1} = \sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{\pm i\phi} = \mp \sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2}$$

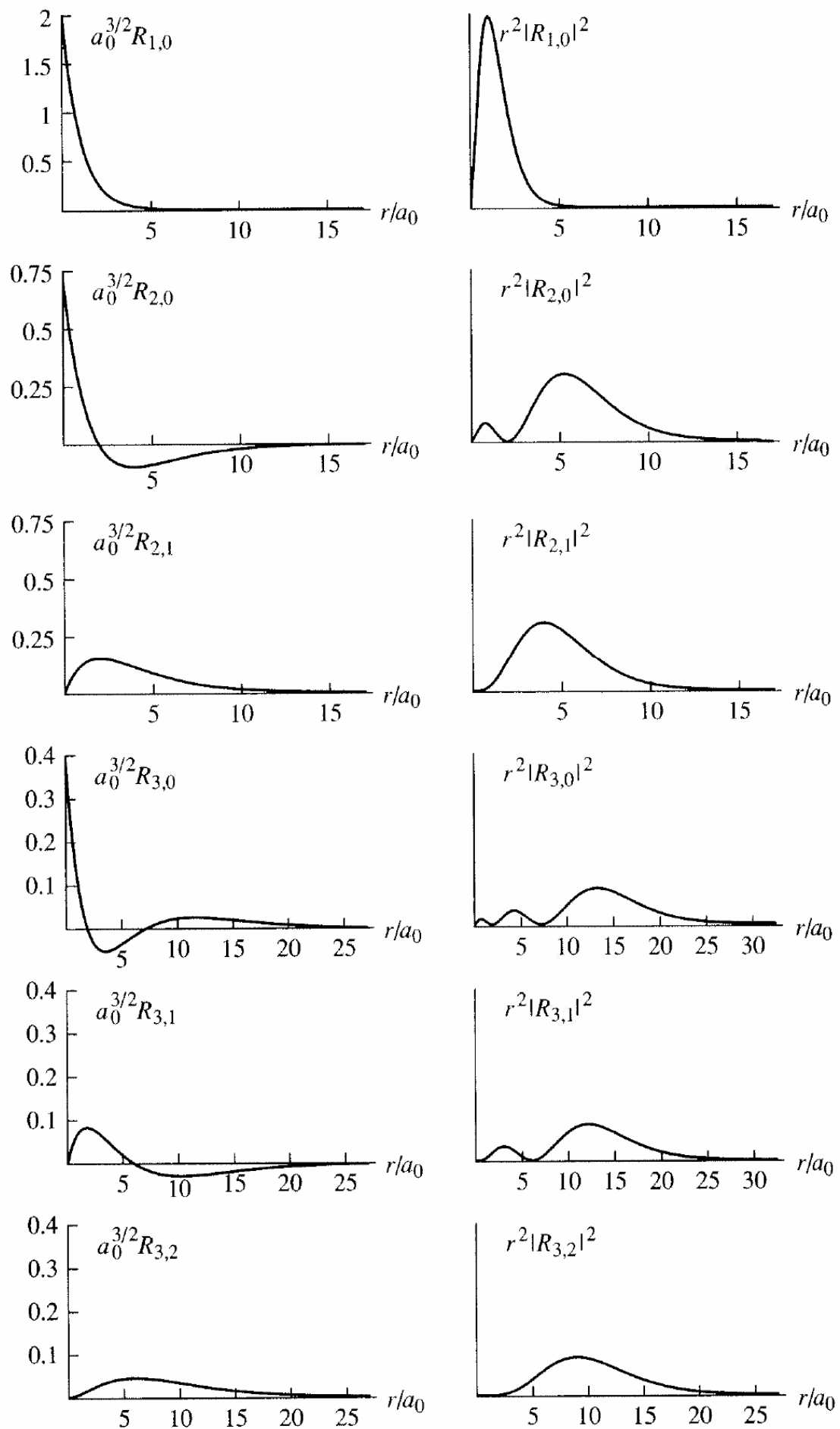
$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi} = \sqrt{\frac{15}{32\pi}} \frac{x^2 - y^2 \pm 2ixy}{r^2}$$

osv



**FIGURE 9.11**  
Plots of  $|Y_{l,m}(\theta, \phi)|^2$  for  $l = 0, 1, 2,$  and  $3$ .





**FIGURE 10.5**

Plots of the radial wave function  $R_{n,l}(r)$  and the radial probability density  $r^2 |R_{n,l}(r)|^2$  for the wave functions in (10.43), (10.44), and (10.45).

# Spektrallinjer

Redan på 1800-talet kände man till att väte emitterar ljus endast med våglängder

$$\frac{1}{\lambda} = R_H \left( \frac{1}{4} - \frac{1}{n^2} \right), \quad n = 3, 4, 5, \dots, \quad R_H \approx 10^7 \text{ m}^{-1}$$

Detta är den så kallade Balmerserien för den synliga delen av vätes spektrum.

Denna egenskap förklaras inom kvantmekaniken:

Om en elektron övergår från  $n_i \rightarrow n_f$  och sänder ut energi i form av en foton med energi

$$E = E_i - E_f = - \frac{m e^4}{2(4\pi\epsilon_0)^2 \hbar^2} \left[ \frac{1}{n_i^2} - \frac{1}{n_f^2} \right] = h f = \frac{h c}{\lambda}$$

$$\Rightarrow \frac{1}{\lambda} = \frac{E}{h c} = \frac{m e^4}{2(4\pi\epsilon_0)^2 \hbar^2 h c} \left[ \frac{1}{n_f^2} - \frac{1}{n_i^2} \right]$$

$\underbrace{\hspace{10em}}_{= 1.097 \cdot 10^7 \text{ m}^{-1}}$

Detta samman ser man formeln ovan med  $n_f = 2$ ,  
 $n_i = 3, 4, 5, \dots$  Detta är Balmerserien, synligt ljus.  
 $n_f = 1$ : Lymanserien, UV ljus  
 $n_f = 3$ : Paschenserien, IR ljus

Detta var en bevisning för den nya kvantmekaniken.