ATOMIC PHYSICS

"kingdom of control"

→ control on the internal state of the atom

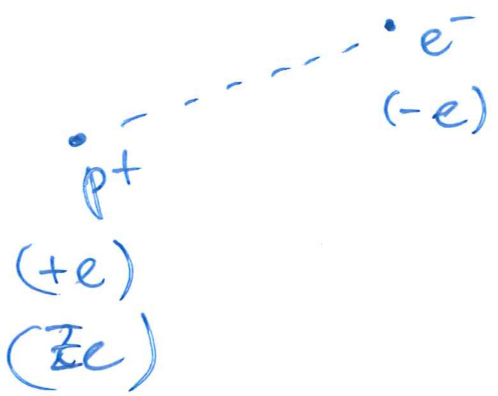
- most precise measurements in physics ⇒ quantum metrology
- quantum information processing ⇒ quantum computing
- quantum optics

→ control of the motional state of atoms

- coldest matter in the universe BEC
- controlling the many-body state of a system

↳ "quantum simulation"

Hydrogen atom : main structure (Schrödinger's theory)



$$E = \frac{1}{2} m \dot{\vec{r}}_1^{\,2} + \frac{1}{2} M \dot{\vec{r}}_2^{\,2} - \frac{e^2\,(Z)}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{R} = \frac{m\vec{r}_1 + M\vec{r}_2}{m_1 + M}$$

$$\vec{p} = \mu \dot{\vec{r}} \qquad \vec{P} = (M+m)\dot{\vec{R}}$$

$$\mu = \frac{mM}{m+M}$$

$$= \frac{1}{2}\mu \dot{\vec{r}}^{\,2} + \frac{1}{2}(M+m)\dot{\vec{R}}^{\,2} - \frac{e^2}{4\pi\epsilon_0 r}$$

$$\mathcal{H} = \frac{\vec{p}^{\,2}}{2\mu} + \frac{\vec{P}^{\,2}}{2(M+m)} - \frac{e^2}{4\pi\epsilon_0 r}$$

$\hat{p}_\alpha$ $\quad \hat{r}_\alpha$

$\alpha = x, y, z$

$$\boxed{[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\,\delta_{\alpha\beta}}$$

$$\hat{\mathcal{H}} = \frac{\hat{\vec{p}}^{\,2}}{2\mu} + \frac{\hat{\vec{P}}^{\,2}}{2(M+m)} - \widehat{\left(\frac{e^2}{4\pi\epsilon_0 r}\right)} \qquad r = |\vec{r}|$$

rest frame of the C.O.M. $\quad \vec{P}^{\,2} = 0$

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0 r}$$

$\vec{r} = 0$

Spherical symmetry

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

$$\langle \vec{r} | \hat{H} | \psi \rangle = \langle \vec{r} | E | \psi \rangle$$

$$\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$$

$$\left[-\frac{\hbar^2}{2\mu} \vec{\nabla}^2 - \frac{e^2}{4\pi\epsilon_0 r} \right] \psi(\vec{r}) = E\,\psi(\vec{r})$$

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

$$\psi(\vec{r}) \longrightarrow \psi(r, \vartheta, \phi)$$

$$\vec{\nabla}^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,\cdot) + \frac{1}{r^2}\overbrace{\left[\frac{1}{\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta \frac{\partial}{\partial\vartheta}(\cdot) \right) + \frac{1}{\sin^2\vartheta}\frac{\partial^2}{\partial\phi^2} \right]}^{*}$$

$$\vec{L} = \vec{r} \times \vec{p} \quad \rightarrow \quad \hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

$$\rightarrow -i\hbar \left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y},\ z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z},\ x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right)$$

$$\vec{L}^2 \rightarrow -\hbar^2 \left[* \right]$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\,\cdot) + \frac{\hat{\vec{L}}^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right] \psi(\vec{r}) = E\psi(\vec{r})$$

$$[\hat{\vec{L}}^2, \hat{\mathcal{H}}] = 0 \qquad [\hat{L}^z, \hat{\mathcal{H}}] = 0$$

Angular momentum in QM

$$\hat{\vec{L}} \qquad [\hat{L}^\alpha, \hat{L}^\beta] = i\hbar \sum_\gamma \epsilon^{\alpha\beta\gamma} \hat{L}^\gamma$$

$$\epsilon^{\alpha\beta\gamma} = \begin{cases} +1 & \text{if } \alpha\beta\gamma \text{ is an EVEN permutation of } xyz \\ -1 & \text{" " ODD "} \\ 0 & \text{otherwise} \end{cases}$$

$\alpha, \beta = x, y, z$

$$[\hat{\vec{L}}^2, \hat{L}^\alpha] = 0$$

$$|lm\rangle \qquad \begin{cases} \hat{\vec{L}}^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle \\ \hat{L}^z |lm\rangle = \hbar m |lm\rangle \end{cases} \qquad \begin{cases} l = 0, 1, 2, \ldots \\ -l \le m \le l \end{cases}$$

$$\hat{L}^\pm = \hat{L}^x \pm i \hat{L}^y \qquad \hat{L}^\pm |lm\rangle = \sqrt{l(l+1) - m(m\pm 1)}\, |l, m\pm 1\rangle$$

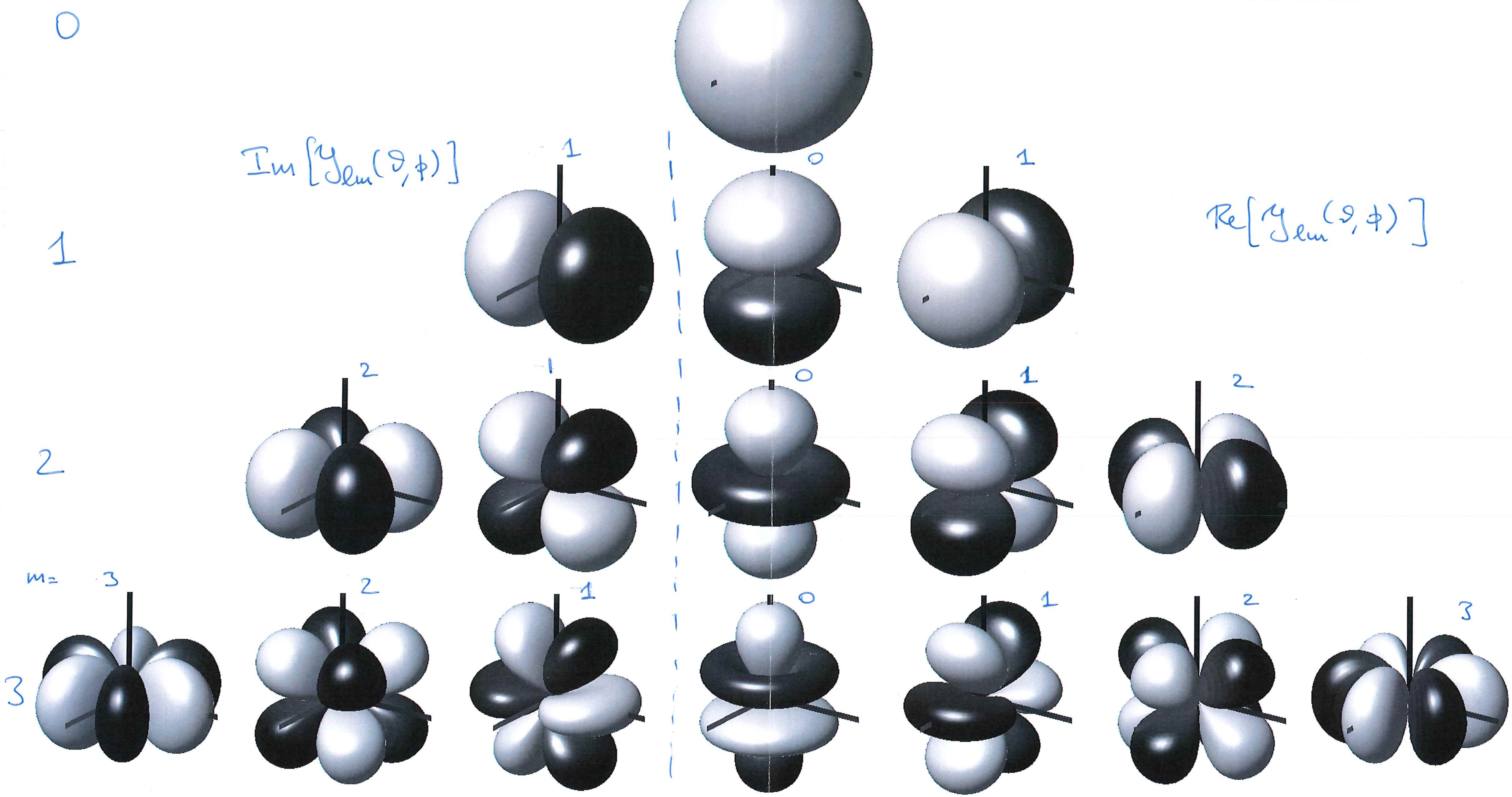
$$\hat{L}^z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\langle \vartheta \phi | lm \rangle = Y_{lm}(\vartheta, \phi) = \frac{e^{im\phi}}{\sqrt{2\pi}} \Theta_{lm}(\vartheta)$$

Spherical Harmonics

$$Y_{00} = \frac{1}{\sqrt{4\pi}} \qquad Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\vartheta \qquad Y_{1,\pm 1} = e^{\pm i\phi} \sqrt{\frac{3}{8\pi}} \sin\vartheta \qquad \ldots$$

SPHERICAL HARMONICS



$$Y^{*}_{\ell m}(\vartheta, \phi) = Y_{\ell, -m}(\vartheta, \phi)$$

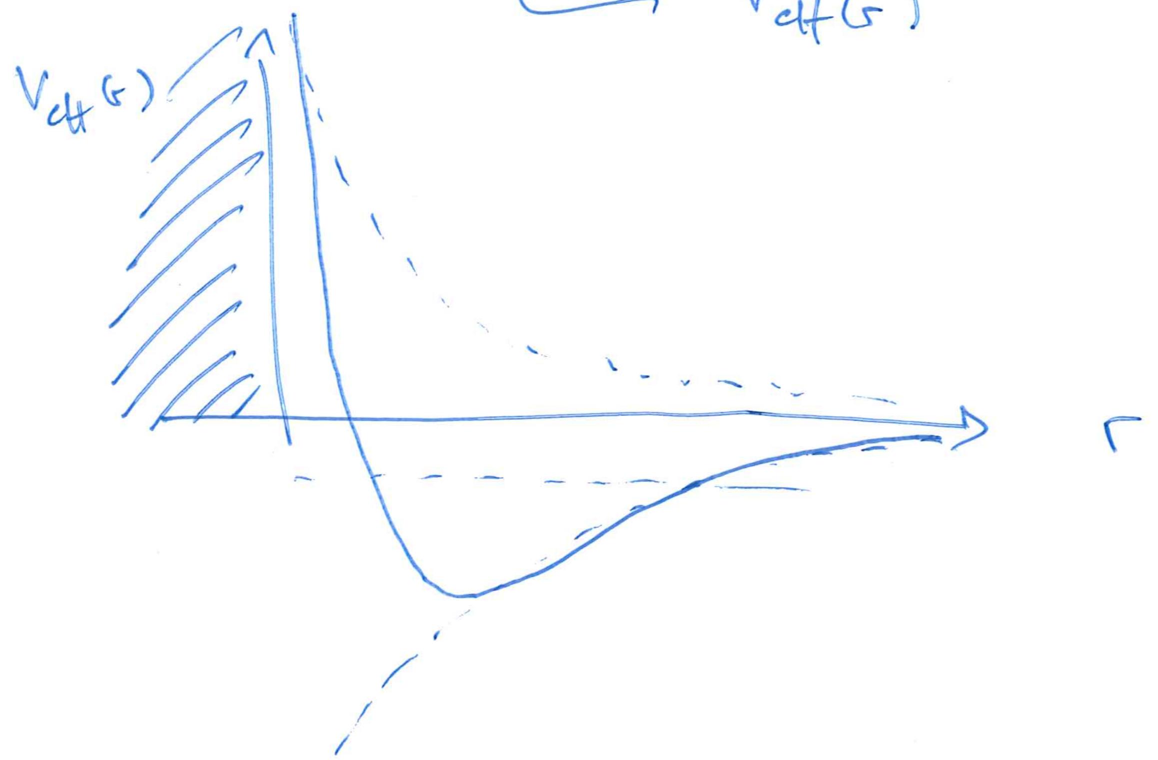
$[\mathcal{H}, \hat{L}^2] = 0 \quad [\hat{\mathcal{H}}, \hat{L}_z] = 0$

$$\psi(\vec{r}) = R_{nl}(r)\, Y_{lm}(\vartheta, \phi)$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}(r\,\cdot) + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{e^2}{4\pi\varepsilon_0 r}\right] R_{nl}(r) = E_{nl} R_{nl}(r)$$

$$R_{nl}(r) = \frac{u_{nl}(r)}{r}$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \underbrace{\frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{e^2 (Z)}{4\pi\varepsilon_0 r}}_{V_{eff}(r)}\right] u_{nl} = E_{nl} u_{nl}$$



$\underline{r \geq 0}$

Natural physical units

Bohr radius $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2 (Z)} \underset{Z=1}{\cong} 0.5\ \text{Å} = 0.5\times10^{-10}\ m$

Rydberg $R_y = \frac{\hbar^2}{2\mu a_0^2} = 13.6\ eV = 13.6 \times 1.6\times10^{-19}\ J$

$\rho = r/a_0 \qquad \epsilon = E/R_y$

$v(\rho) = u(\rho a_0)$

$$\left[-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{2}{\rho} \right] v_{n\ell}(\rho) = \epsilon_{n\ell}\, v_{n\ell}(\rho)$$

$\underline{\rho \to 0}$ $\qquad$ $\underline{\rho \to \infty}$ $\qquad$ Bound states : $\epsilon_{n\ell} < 0$

$\downarrow$ $\qquad$ $\searrow$

$\underline{v_{n\ell} \sim \rho^{\ell+1}}$ $\qquad$ $\underline{v_{n\ell} \sim e^{-\rho/\lambda_{n\ell}}}$ $\qquad$ $\lambda_{n\ell} = \frac{1}{\sqrt{|\epsilon_{n\ell}|}}$

$$v_{n\ell} = f_{n\ell}(\rho)\, e^{-\rho/\lambda_{n\ell}}$$

$\rho' = \frac{2}{\lambda}\rho$

$$\left[\frac{d^2}{d\rho'^2} + \frac{2}{\lambda}\frac{d}{d\rho'} + \frac{\ell(\ell+1)}{\rho'^2} - \frac{2}{\rho'} \right] f_{n\ell}(\rho') = 0$$

$$f_{n\ell}(\rho') = \underline{\underline{(\rho')^{\ell+1}}} \underbrace{\sum_{k=0}^{\infty} c_k (\rho')^k}_{g(\rho')} \qquad k_{max} < \infty$$

$$\left[\rho' \frac{d^2}{d(\rho')^2} + (2\ell + 2 - \rho') \frac{d}{d\rho'} + (\lambda_{n\ell} - \ell - 1)\right] g = 0$$

$$k_{max} + \ell + 1 = \lambda_{n\ell} \qquad \underline{\lambda_{n\ell} = n} = 1, 2, \ldots$$ principal quantum number

$$\boxed{\ell \leq n-1}$$

$$\lambda_{n\ell}^2 = \frac{1}{|\epsilon_{n\ell}|} = n^2 \qquad \boxed{E_{n\ell} = E_n = -\frac{R_y}{n^2}}$$

$$\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r)\, Y_{\ell m}(\theta, \phi) \rightarrow E_n$$

9

4

Degeneracy
$g_n = n^2$

1

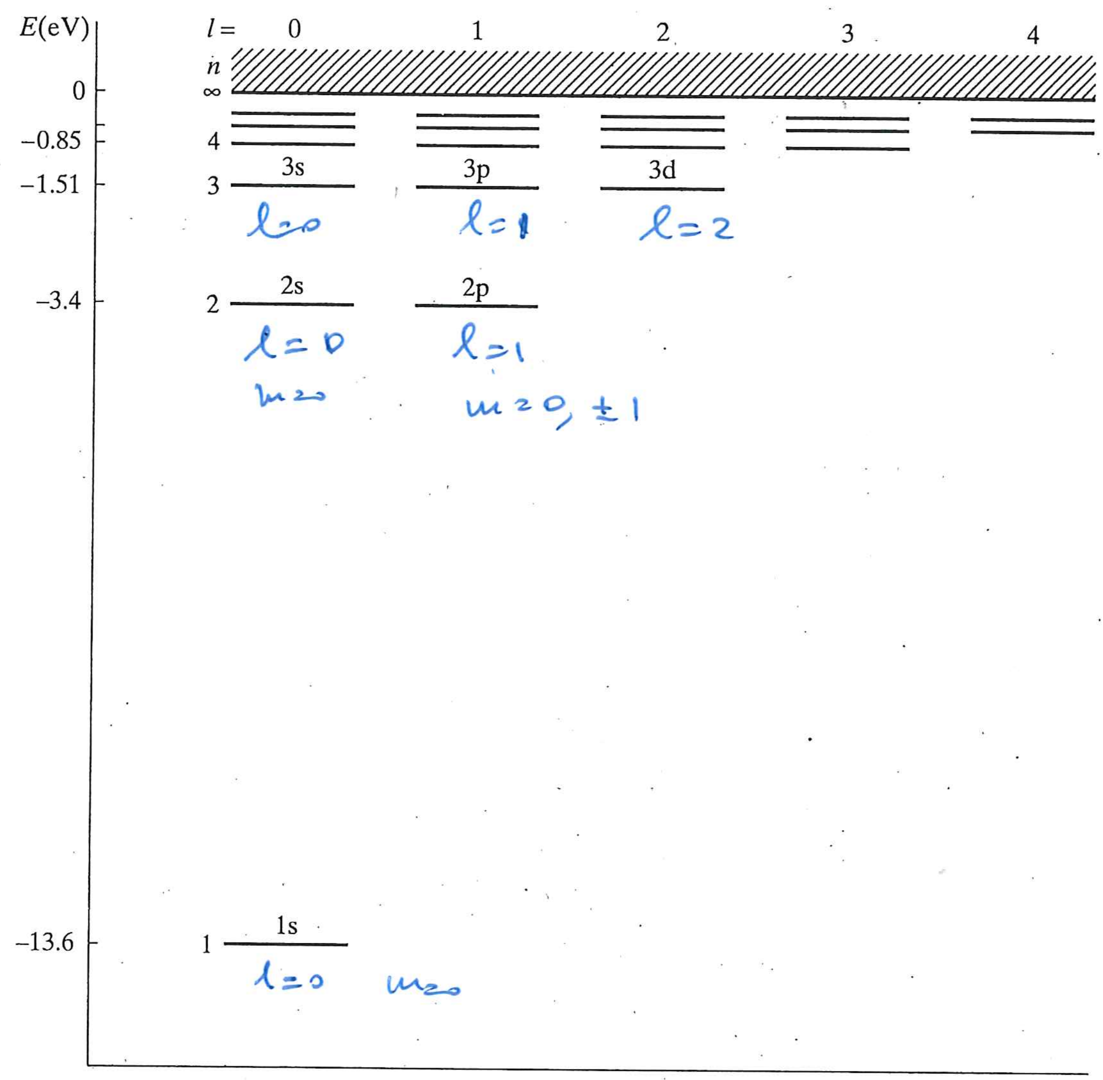


Figure 3.2 Energy-level diagram for atomic hydrogen.

Having obtained the energy levels of one-electron atoms within the framework of the Schrödinger non-relativistic theory, we may now ask about the spectral lines corresponding to transitions from one level to another. This problem will be discussed in detail in the next chapter, where we shall study the interaction of one-electron atoms with electromagnetic radiation. In particular, we shall calculate the transition rates for the most common transitions, the so-called electric dipole transitions, and we shall prove that these transitions obey the selection rules

$$\begin{aligned} \Delta l &= l - l' = \pm 1 \\ \Delta m &= m - m' = 0, \pm 1 \end{aligned} \tag{3.33}$$

while $\Delta n = n - n'$ is arbitrary. Here the symbols n, l, m refer to the quantum numbers of the upper state and n', l', m' to those of the lower state of the transition. Since the bound state energies E_n depend only on n, and because transitions can occur between states with any two values of n, it is clear that the Bohr frequency

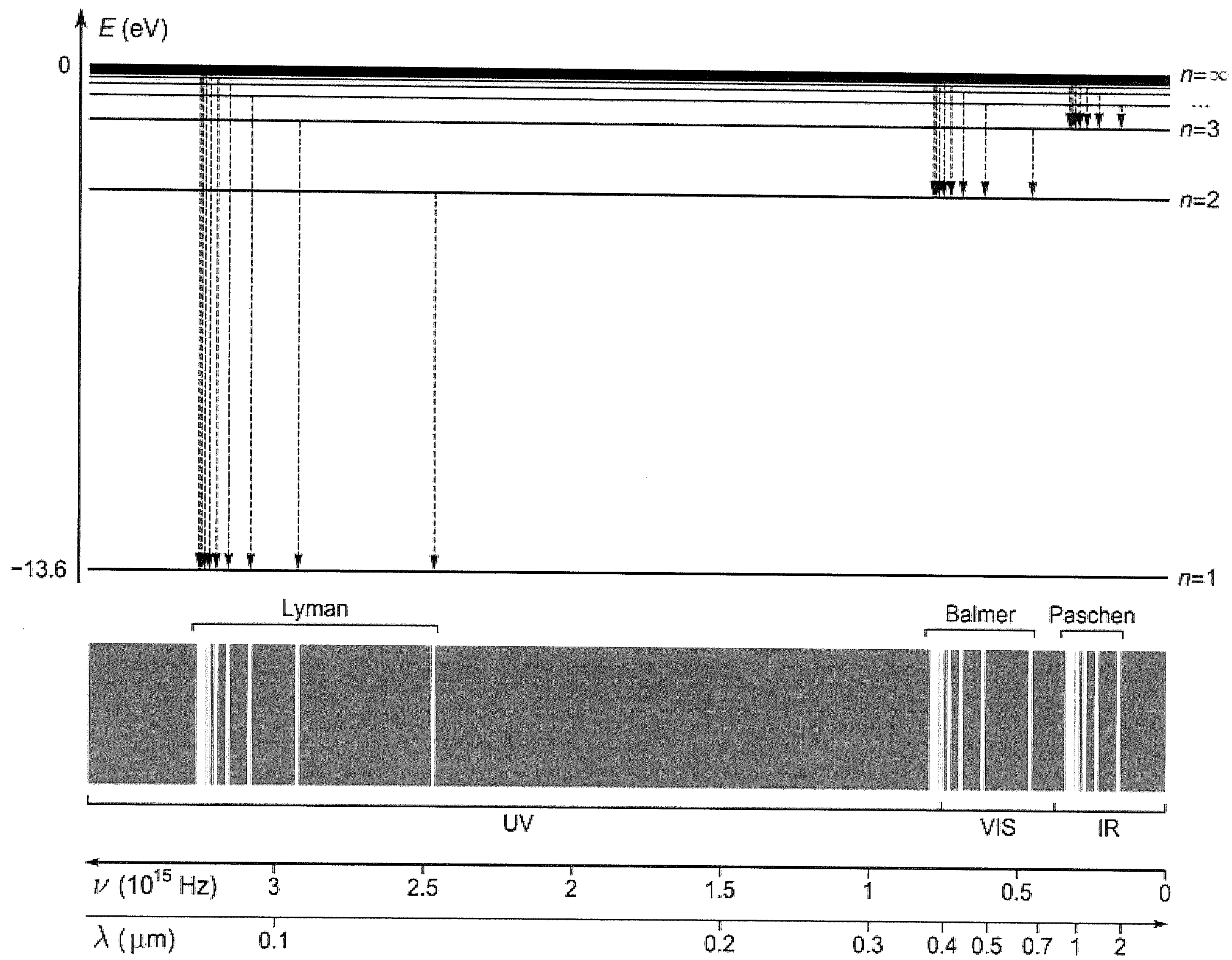


Fig. 1.2 Scheme of hydrogen levels and different groups of transitions: Lyman (in the ultraviolet), Balmer (largely in the visible spectrum) and Paschen (in the infrared).

nl = 10

20

21

30

31

32

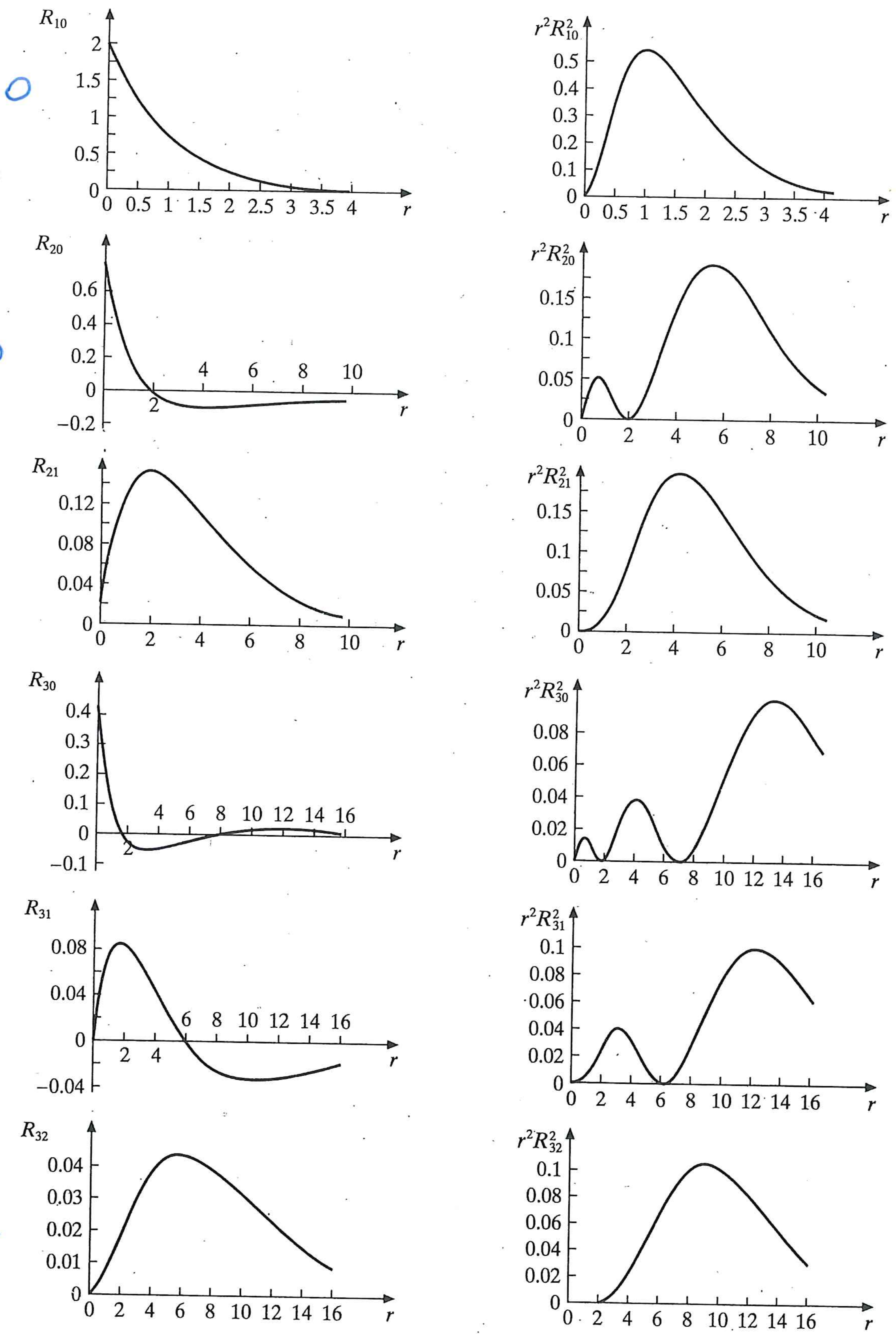
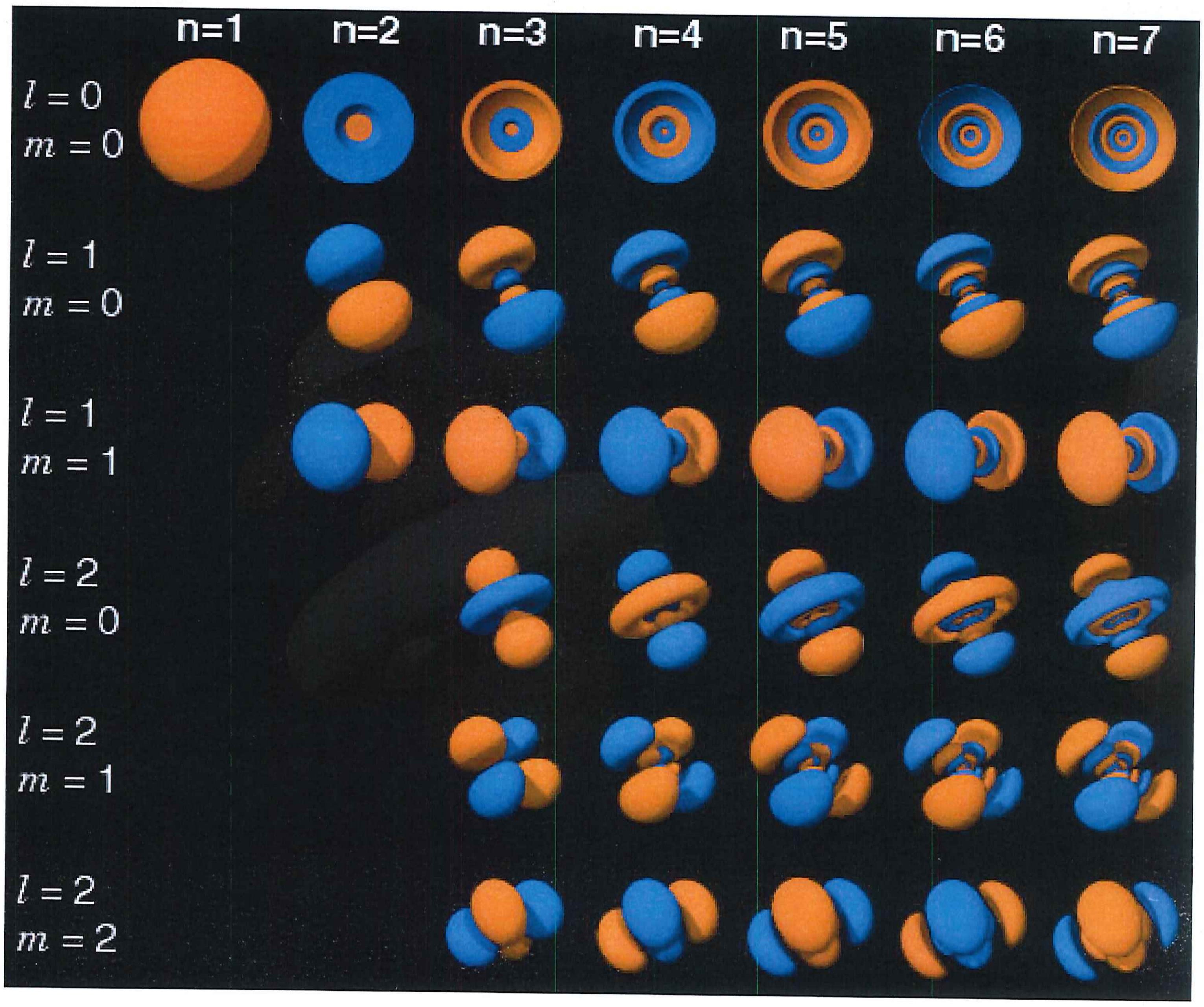


Figure 3.3 Radial functions $R_{nl}(r)$ and radial distribution functions $r^2R_{nl}^2(r)$ for atomic hydrogen.


n=1
n=2
n=3
n=4
n=5
n=6
n=7
l = 0 m = 0
l = 1 m = 0
l = 1 m = 1
l = 2 m = 0
l = 2 m = 1
l = 2 m = 2

$$f_{nl} = \text{poly}(l+1+k_{max}) \qquad k_{max} = n-l-1$$
$$= \text{poly}(n)$$

$$R_{nl}(r) = \frac{u_{nl}}{r} = N \frac{e^{-\frac{r}{na_0}}}{r} \underbrace{\left(\frac{r}{a_0}\right)^{l} L^{2l+1}_{n+l}\left(\frac{r}{a_0}\right)}_{\text{poly}(n)} = \underbrace{e^{-\frac{r}{na_0}} \cdot \text{poly}(n-1)}$$

Relativistic effects in the H atom : fine-structure of H

P.A.M. Dirac : Dirac's theory

$\vec{S}$ e^-

$\exists\ p^+$

$$[\hat{S}^\alpha, \hat{S}^\beta] = i\hbar \sum_{\alpha\beta\gamma} \epsilon_{\alpha\beta\gamma} \hat{S}^\gamma$$

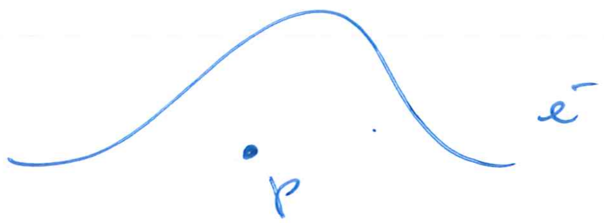
intrinsic (spin) angular momentum

$$l \rightarrow \underline{s = \tfrac{1}{2}}$$

$$\vec{m} = -\frac{g\mu_B}{\hbar}\vec{S} \qquad \text{magnetic moment}$$

$$g \simeq 2$$

$$\mu_B = \frac{e\hbar}{2m} \qquad \text{Bohr's magneton}$$
$$= 9.27 \times 10^{-24}\ J/T$$



$$\Delta x \to \Delta p \simeq \frac{\hbar}{\Delta x} \qquad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m e^2}$$

$$\frac{v}{c} \sim \frac{\Delta p}{mc} \sim \frac{\hbar}{m a_0 c} = \alpha \simeq \frac{1}{137}$$

fine structure constant

$$= \frac{e^2}{4\pi\epsilon_0 \hbar c}$$

$$E_n' = E_n + \underset{\uparrow}{\zeta\,\alpha^2} + O(\alpha^4) \; - -$$

$$\mathcal{H}' = \mathcal{H} + \overbrace{\mathcal{H}_{so} + \mathcal{H}_{rel} + \mathcal{H}_D} + \ldots$$

$\mathcal{H}_{so}$: spin-orbit coupling

$\mathcal{H}_{rel}$: relativistic correction to the kinetic energy

$\mathcal{H}_D$: Darwin term