Problems:

8.14, 8.16, 8.17, 8.18, 8.22, 8.25, 8.24, 8.26, 8.29, 9.21

- Show that the $2p$ wave functions of the hydrogen atom satisfy the radial Schrödinger equation.
- Show that $Y_{10}(\theta, \phi)$ has angular momentum momentum squared $2\hbar^2$ as in Eq. 4
- Show that $Y_{11}(\theta, \phi)$ has z component of angular momentum $\hbar$ as in Eq. 6
- What is the electronic structure of Ne. Make an educated guess about its chemical reactivity.

Wave Functions symmetric potential

- The wave fuctions in a radial symmetric potential (for example $-k_C e^2/r$) can be written

$$\psi_{n\ell m}(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \tag{1}$$

  with $R_{n\ell}$ the radial wave function and $Y_{\ell m}$ the sphereical harmonics

- In general the wave functions are characterized by the three quantum numers
  - The radial quantum number

$$n = 1, 2, 3, 4 \ldots \tag{2}$$

    which labels the radial excitation.
  - The angular momentum quantum number

$$\ell = 0, 1, \ldots n - 1 \tag{3}$$

    which labels the total angular momentum of this wave functions. These wave functions have definite angular momentum $\ell(\ell+1)\hbar^2$

$$\mathbb{L}^2 Y_{\ell m} = \ell(\ell+1)\hbar^2 \, Y_{\ell m} \tag{4}$$

    These are for $\ell = 0, 1, 2, 3, 4 \ldots$ also called by the names

$$\ell = s, p, d, f, g \tag{5}$$

    i.e. an "s-wave" is another name for the $\ell = 0$ wave function.
  - And a magnetic quantum number. These wave functions have definite z component of angular moemntum $m\,\hbar$

$$\mathbb{L}_z Y_{\ell m} = m\hbar \, Y_{\ell m} \tag{6}$$

    with

$$m = -\ell \ldots \ell \tag{7}$$

- The angular momentum operators are

$$\mathbb{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \frac{\cos(\theta)}{\sin(\theta)} \frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial\phi^2} \right) \tag{8}$$

$$\mathbb{L}_z = -i\hbar \frac{\partial}{\partial\phi} \tag{9}$$

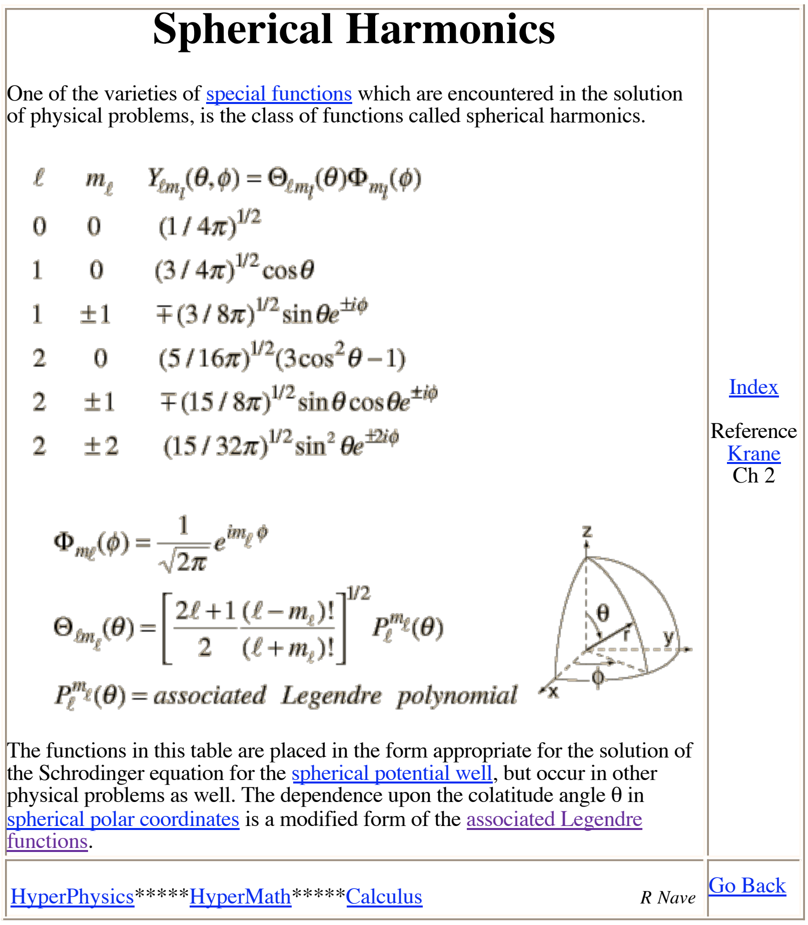
- The lowest angular wave functions are given on the next page

Hydrogen Atom

- For the special case of the hydrogen atom the potential $V(r)$ is just the Coulomb potential

$$V(r) = -\frac{k_C e^2}{r} \tag{10}$$

  and the lowest radial wave functions are given on the next page for $n = 1$ and $n = 2$ and the corresponding ℓ.



Spherical Harmonics

One of the varieties of special functions which are encountered in the solution of physical problems, is the class of functions called spherical harmonics.

ℓ	m_ℓ	$Y_{\ell m_\ell}(\theta,\phi)=\Theta_{\ell m_\ell}(\theta)\Phi_{m_\ell}(\phi)$
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2}\cos\theta$
1	±1	$\mp(3/8\pi)^{1/2}\sin\theta e^{\pm i\phi}$
2	0	$(5/16\pi)^{1/2}(3\cos^2\theta-1)$
2	±1	$\mp(15/8\pi)^{1/2}\sin\theta\cos\theta e^{\pm i\phi}$
2	±2	$(15/32\pi)^{1/2}\sin^2\theta e^{\pm 2i\phi}$

$$\Phi_{m_\ell}(\phi)=\frac{1}{\sqrt{2\pi}}e^{im_\ell\phi}$$

$$\Theta_{\ell m_\ell}(\theta)=\left[\frac{2\ell+1}{2}\frac{(\ell-m_\ell)!}{(\ell+m_\ell)!}\right]^{1/2}P_\ell^{m_\ell}(\theta)$$

$$P_\ell^{m_\ell}(\theta)=associated\ \ Legendre\ \ polynomial$$

The functions in this table are placed in the form appropriate for the solution of the Schrodinger equation for the spherical potential well, but occur in other physical problems as well. The dependence upon the colatitude angle θ in spherical polar coordinates is a modified form of the associated Legendre functions.

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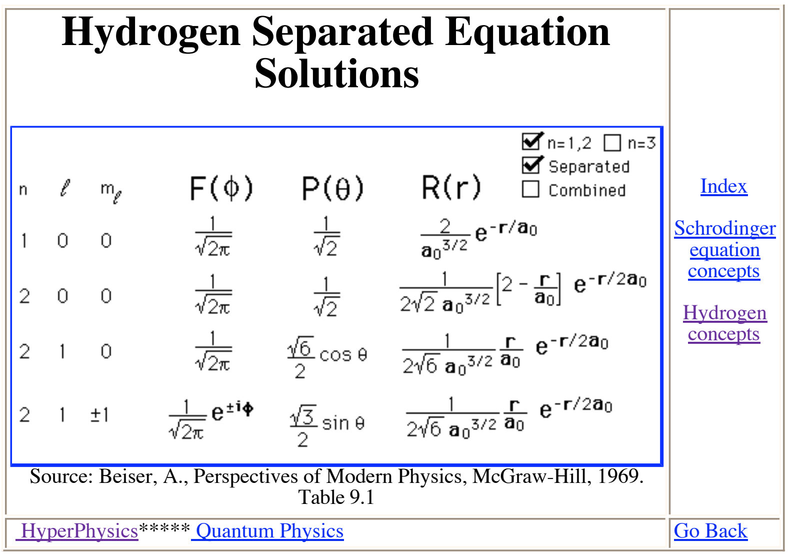

Hydrogen Separated Equation Solutions

☑ n=1,2 ☐ n=3
☑ Separated
☐ Combined

n	ℓ	m_ℓ	F(ϕ)	P(θ)	R(r)
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{a_0^{3/2}}e^{-r/a_0}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}\,a_0^{3/2}}\left[2-\frac{r}{a_0}\right]e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2}\cos\theta$	$\frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$
2	1	±1	$\frac{1}{\sqrt{2\pi}}e^{\pm i\phi}$	$\frac{\sqrt{3}}{2}\sin\theta$	$\frac{1}{2\sqrt{6}\,a_0^{3/2}}\frac{r}{a_0}e^{-r/2a_0}$

Source: Beiser, A., Perspectives of Modern Physics, McGraw-Hill, 1969. Table 9.1

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FIG. 1: The hydrogen wave functions. The full wavefunction is $\psi_{nlm}=F_m(\phi)P_{\ell m}(\theta)R_{n\ell}(r)$

- The energies are
$$E_{n\ell} = -\frac{\hbar^2}{2ma_0^2}\frac{Z^2}{n^2} = -\frac{k_C e^2}{2a_0}\,\frac{Z^2}{n^2} \tag{11}$$
- The radial wave functions for the hydrogen atom are given on below

Radial Schrödinger Equation

- Its useful to define a radial wave function
$$u_{n\ell}(r) \equiv rR_{n\ell}(r)$$
(The book is the only one I know of which calls this $g(r)$). This is useful because if the Schrödinger equation is is written down with a wave function of the form given above, it reduces to the radial Schrödinger equation
$$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)\hbar^2}{2mr^2} + V(r)\right] u_{nl} = E_{nl} u_{nl} \tag{12}$$
for s-wave states (i.e. $\ell = 0$), this is the same as a one dimensional Schrödinger equation.
- For a classical particle going moving around a central potential the kinetic energy is
$$KE = \frac{p_r^2}{2M} + \frac{L^2}{2Mr^2} \tag{13}$$
with L the angular momentum. You should feel comfotable deriving this for classical motion. You should understand that the r-derivative terms correspond to the radial kinetic energy $p_r^2/2m$, while the $\ell(\ell+1)$ term corresponds to the angular kinetic energy $L^2/(2mr^2)$.
- You should be able to verify that this or that functions satisfies the radial Schrödinger equation.

Probability Distribution

- The probability that the wave function be in a certain region of size dV is
$$P(x,y,z)\,dV = |\psi(x,y,z)|^2\ dV \tag{14}$$
- For an electron in a spherically symmetric potential, the probability to find an electron between r and $r+dr$
$$P(r)\,dr = |rR(r)|^2\,dr = |u_{n\ell}(r)|^2\,dr \tag{15}$$
It is normalized to one
$$\int_0^\infty P(r)dr = \int_0^\infty |u_{n\ell}(r)|^2 = 1 \tag{16}$$
- This probability distribution can be used to find the probability that the electron is between this radius and that, or the most likely value radius (maximum probability).
- It can be used to find average quantities. For instance
  - the average radius is
$$\bar{r} = \langle r \rangle = \int_0^\infty r|u_{n\ell}(r)|^2 \tag{17}$$
  - The average potential enenergy is for the hydrogen atom is
$$\langle V(r) \rangle \ = \int_0^\infty -\frac{k_C e^2}{r}\,|u_{n\ell}(r)|^2 \tag{18}$$
  - The variance in the radius is
$$(\Delta r)^2 = \left\langle r^2 \right\rangle - \langle r \rangle^2 \tag{19}$$
  - The average kinetic energy is
$$\langle KE \rangle = \int_0^\infty u_{n\ell}(r)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\ell(\ell+1)\hbar^2}{2Mr^2}\right] u_{n\ell}(r) \tag{20}$$