\[ \int_0^{2\pi} d\phi \int_0^\pi d\theta \, Y_{l m}^* (\theta, \phi) \, Y_{l' m'} (\theta, \phi) = C_S_{l, m} \, S_{m, m'} \]

Radial Equation Next Time

\[ 10/6/04 \]

\[ \int_0^{2\pi} d\phi \int_0^\pi d\theta \, \sin \theta \, Y_{l m}^* Y_{l m'} = 0 \quad \text{if } l \neq l' \text{ or } m \neq m' \]

Radial Equation

\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \ell (\ell + 1) \frac{1}{r^2} + \frac{2m}{\hbar^2} \left( E - \frac{2e^2}{r} \right) R = 0 \]

Physical Boundary Conditions

\[ R(r) \to 0 \quad \text{as} \quad r \to \infty \]

At large \( r \)

\[ \frac{1}{r^2} \left( 2r \frac{dR}{dr} + r^2 \frac{d^2R}{dr^2} \right) + \ell (\ell + 1) \frac{1}{r^2} + \frac{2m}{\hbar^2} \left( E - \frac{2e^2}{r} \right) \to 0 \]

\[ \frac{d^2R}{dr^2} + \frac{2m}{\hbar^2} E(R) = 0 \Rightarrow R(r) = e^{-\gamma} \]

\[ \gamma = \frac{-2mE}{\hbar^2} \]

\[ E < 0 \]
In general \( R(r) = \text{const} \left[ \sum_{n} b_n r^n c^{-n^2} \right] \)

Even near zero

\[
\frac{\hbar^2 \frac{Z^2 e^2}{r^2}}{2m} = \text{integer} = n^2
\]

\( n = l+1, l+2, \ldots \)

\( l = n-1, n-2, \ldots \)

\[
\left( \frac{\hbar^2 \frac{Z^2 e^2}{r^2}}{2m} \right)^2 \frac{1}{n^2} = -\frac{2\hbar^2 E_n}{n^2}
\]

\[
E_n = -\frac{\hbar^2 \frac{Z^2 e^4}{2m^2}}{2} \left( \frac{1}{n^2} \right)
\]

Similiar to the Bohr model

In this, electron is distributed over space, while in Bohr model, \( e^- \) has well-defined orbit.
\[ R_{10}(r) = \cdots \frac{2^{2}}{a_0} e^{-\frac{2r}{a_0}} \quad a_0 \text{ is Bohr Radius} \]
\[ R_{20}(r) = \cdots \left(2 - \frac{2r}{a_0}\right) e^{-\frac{2r}{a_0}} \]
\[ R_{21}(r) = \cdots \left(\frac{2r}{a_0}\right) e^{-\frac{2r}{2a_0}} \]

Normalization Constant

Summary:

\[ f(r, \theta, \phi) = R_{n\ell}(r) Y_{\ell m}(\theta, \phi) \]

Projection of angular momentum onto some symmetry axis. Azimuthal principle.

<table>
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<th>( n )</th>
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<th>2</th>
<th>3</th>
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<tr>
<td></td>
<td>-2</td>
<td></td>
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</tbody>
</table>

The number of states is 3, 1, 5, 8, 3, and energy is independent of \( m, \ell \), so each of these are degenerate.

\[ g_n = \text{Degeneracy} = n^2 \]
Orbitals & Radial Distribution

- The probability density for finding an electron between \( r \) and \( r + dr \) is

\[
\psi^*(r) \psi(r) \, dr
\]

Probability of finding an electron is \( |\psi(r)|^2 \frac{dr}{dA} \) or \( d^3r \)

In spherical coordinates

\[
d^3r = \rho^2 \sin \theta \, d\rho \, d\theta \, d\phi
\]

\[
|\psi_{nm}(\theta, \phi, r)|^2 \rho^2 \sin \theta \, d\rho \, d\theta \, d\phi
\]

Gives probability of finding an electron in some volume \( dr \, d\theta \, d\phi \)

Density between \( r \) to \( R \) to find probability that an electron is located at some distance \( dr \) from the nucleus, we integrate out spatial dependence

\[
L^2 \int_0^\infty \int_0^\pi \int_0^{2\pi} \rho^2 |\psi_{nm}|^2 \sin \theta \ d\rho \ d\theta \ d\phi = 1
\]

\[
\int_0^R \left| \psi_{nm}(r) \right|^2 r^2 \, dr = 1
\]
Most Probable $r$?

Let $n = 1$

$E(r) = a e^{-2r/a_0}$

$P(r) \propto r^2 e^{-2r/a_0}$

$$\langle r \rangle = \int_0^\infty r^2 e^{-2r/a_0} \, dr$$

Average $r$ - Nucleus Distance

Its max. occurs at $\frac{dP}{dr} = 0$ (its maximum)

$$\frac{dP}{dr} = \frac{2}{r} P(r) - \frac{2}{a_0} P(r) \Rightarrow r_{mp} = \frac{a_0}{2}$$

$$\langle r \rangle = \int_0^\infty r^3 e^{-2r/a_0} \, dr$$

$I_n = \int_0^\infty r^n e^{-ar}$

$r^n e^{-ar} = \frac{d^n}{dr^n} d^n e^{-ar}$

$I_n = \int_0^\infty d^n e^{-ar}$

$\frac{d^n}{dr^n} \left( \frac{1}{a} e^{-ar} \right) = \frac{d^n}{dr^n} \left( \frac{1}{a} e^{-ar} \right) \bigg|_0^\infty$

$$\langle r \rangle = \frac{6}{2^{1/2}} \frac{2}{2} = \frac{3}{2} r_{mp} = \langle r \rangle$$
p(r)

S-orbitals

\[ r_{p_{1}}(r) \]

Discrepancy due to that \( p(r) \) goes to 0 as \( r \to \infty \), but never equals 0 (i.e., it is not completely symmetric)

\[ r_{p_{2}}(r) \]

\[ r_{p_{0}}(r) \]

2s

\[ r_{2s} \]

\[ r_{2s}^2 \]

P-orbitals \( \rightarrow l = 1 \Rightarrow m = -1, 0, 1 \)

\( \Phi_{m} \) is complex \( \Phi_{m} \neq \Phi_{-m}^{*} \)

\[ \cos(m\phi) = \frac{1}{2} [ \Phi_{m}(\phi) + \Phi_{-m}^{*}(\phi) ] = \frac{1}{2} [ \Phi_{m}(\phi) + \Phi_{-m}(\phi) ] \]