QM III.

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SZÉCHENYI ISTVÁN EGYETEM SZE - GYŐR

Fizika és Kémia Tanszék

Energy states of electrons in H atom

The electron's potential energy in the electric field of the H atom's nucleus:

$$\boldsymbol{E_p} = -\frac{\boldsymbol{e}^2}{4\pi\varepsilon_0 \boldsymbol{r}},$$

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Since the electric field of the nucleus is spherically symmetric, we look for a spherically symmetric solution $F(r)$ of the equation :

$$\psi(\underline{r}) = F(r).$$

Then the Schrödinger equation is:

$$\frac{d^2F(r)}{dr^2} + \frac{2}{r}\frac{dF(r)}{dr} + \frac{2m_e}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)F(r) = 0.$$

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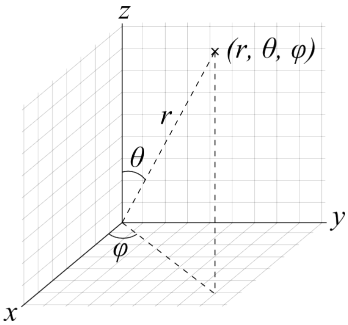
This spherically symmetric solution gives the ground state of the electron in the H atom. Since the nucleus-electron system is bound, the electron can only have discrete energies in the H atom.

The state functions of the excited states are not necessarily spherically symmetric, but can always be written in the following form:

$$\psi(\underline{r}) = \boldsymbol{R_{n,l}(r)} . \boldsymbol{Y_{l,m}}(\theta, \varphi)$$

$\boldsymbol{R_{n,l}(r)}$ - radial function, $\boldsymbol{Y_{l,m}}(\theta, \varphi)$ - spherical function.
$(\boldsymbol{r}, \theta, \varphi)$ the spherical coordinates according to the figure below!



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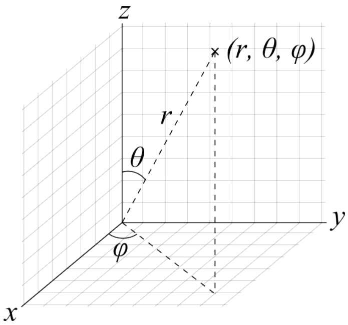


The state of the electron in the H atom is characterized by 3 quantum numbers: (n, l, m).

These respectively determine the magnitude of 3 conserved quantities:

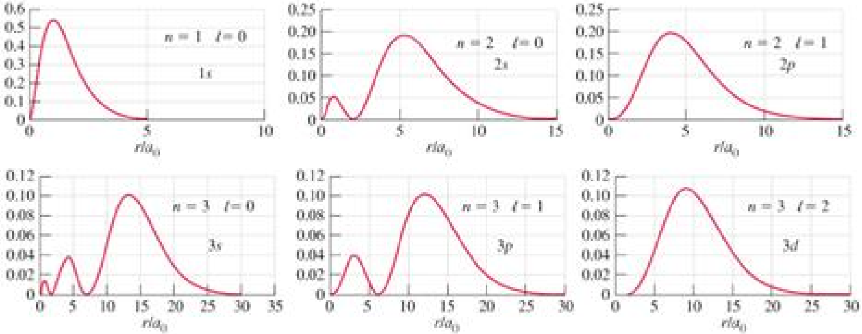
$n = 1, 2, ...$ - main quantum number - determines the discrete total energy of the electron,

$l = 0, 1, ..., n-1$ - secondary quantum number - determines the magnitude of electron's angular momentum,

$m = -l, -l+1, ..., 0, ..., l-1, l$ - magnetic quantum number - determines one component of electron's angular momentum .

$$E_n = \frac{E_1}{n^2} = \frac{-13,41\ eV}{n^2},\ L^2 = l(l+1)\hbar^2,\ L_z = m\hbar$$

Radial functions



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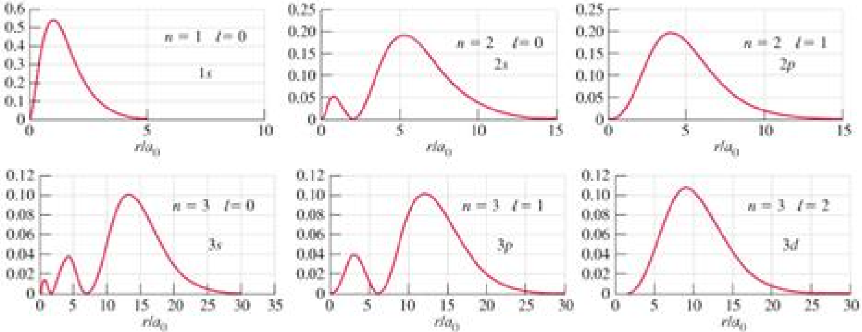
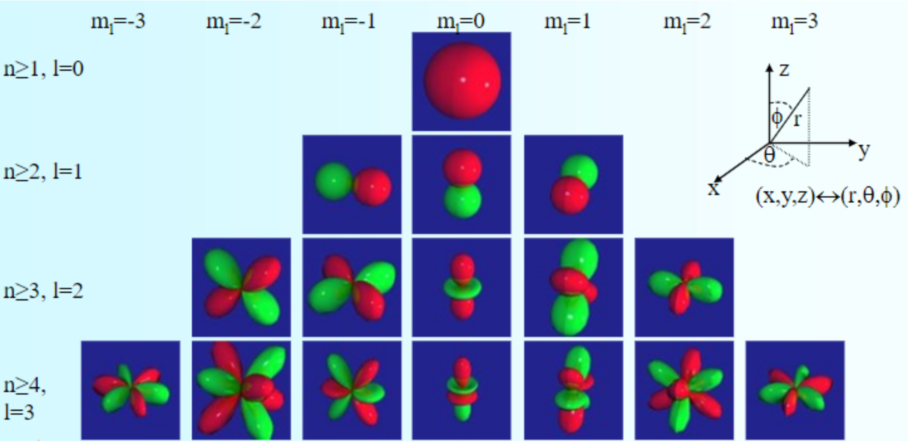


Contours of spherical functions



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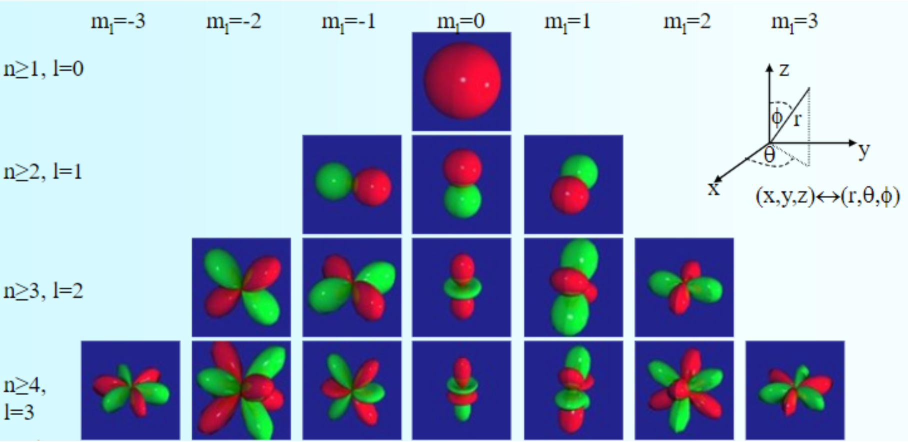

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Larmor-theorem: A charged system with angular momentum has also a magnetic moment.

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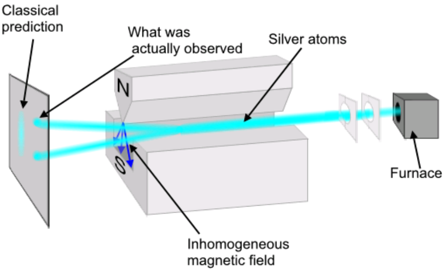

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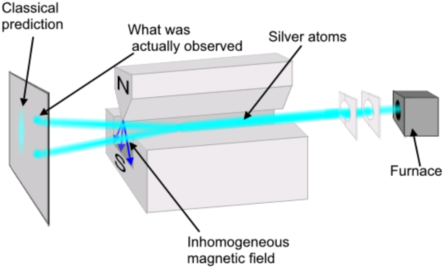

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In addition to the previously mentioned angular momentum, the electron also has an angular momentum of another kind, which cannot be linked to any motion. It is called $\Rightarrow$ Spin.

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Spin is also a quantized quantity. In the case of the electron, it can have two projections for a selected direction.

$$\boldsymbol{S_z = s_z \hbar},$$

where S_z- is a projection of the electronspin, s_z-is the so called spin quantum number, its value can be $+\frac{1}{2}, -\frac{1}{2}$ (s_z is not an integer!).

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The energy minimum principle and the Pauli principle form the basis of the quantum physics' interpretation of the periodic table.

Thank you!