1. Physics 13: Hydrogen atom in QM

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3-dimensional stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)+U(x,y,z)\psi(x,y,z)=E\,\psi(x,y,z)$$

Coulomb potential: $U(r)=-k_{EM}\frac{e^2}{r}$ with $r=\sqrt{x^2+y^2+z^2}$

can change variables to (r,ϑ,φ) so $\psi(r,\vartheta,\varphi)=\mathrm{R(r)}\Theta(\vartheta)\Phi(\varphi)$

3 variables → 3 Quantum Numbers for bound state solutions
n = radial (r) quantum no., l = orbital (θ) q. no.,
m_l = azimuthal (φ) q. no.
(note that spherical symmetry suggests spherical coords)

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2. Radial equation

Radial equation

Using factorized form $\psi(r,\vartheta,\varphi)=\mathrm{R(r)}\Theta(\vartheta)\Phi(\varphi)$

and substituting into the equation → simpler radial equation

$$-\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}\right]R(r)-k_{EM}\frac{e^2}{r}R(r)=ER(r)$$

where l is an integer determined by the angular dependence
and $l = 0,1,2,\ldots$ will all label distinct solutions

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3. Quantum numbers

Quantum numbers

- 3 quantum numbers are related

  $n = 1,2,3,\ldots$

  $l = 0,1,2, \ldots n-1$ n values for each n

  $m_l = -l, -l+1, \ldots, +l-1, +l$ $2l+1$ values for each l
- n= principal q. no. for Coulomb case
- l = orbital q.no. for any central
- m_l = magnetic q.no. force

$L = \sqrt{l(l+1)}\hbar$ Orbital angular momentum

$L_z = m_l\hbar$ for z defined along some $\vec{B}$ or arbitrary

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4. Angular momentum

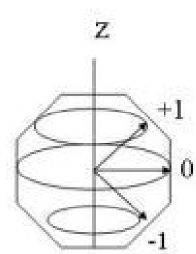
Angular momentum

Then for given L (and l)

$$\frac{L_z}{L} = \cos(\theta_L) = \frac{m_l\hbar}{\sqrt{l(l+1)}\hbar} = \frac{m_l}{\sqrt{l(l+1)}} \quad \text{quantized directions!}$$

example: $l = 1 \rightarrow L\sqrt{2}\hbar$ and $m_l = -1,0,1$

so $\cos(\theta_L) = \frac{-1}{\sqrt{2}}, 0, \frac{+1}{\sqrt{2}}$



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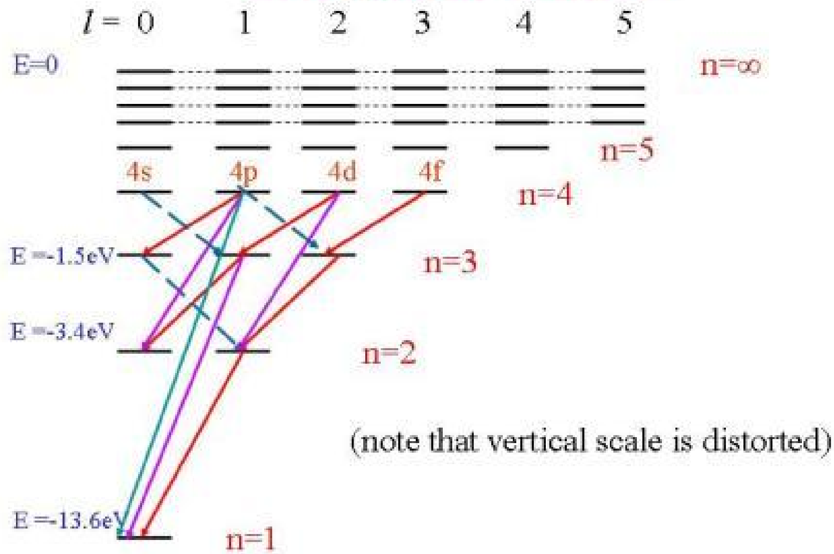
5. Energy level diagram

Energy level diagram



6. Hydrogen wave functions

Hydrogen wave functions

$$\psi_{n,l,m_l}(r,\vartheta,\varphi) = R_{n,l}(r)\Theta_{l,m_l}(\vartheta)\Phi_{m_l}(\varphi)$$

Ground state: $n = 1 \Rightarrow l = 0, m_l = 0$

$$\psi_{1,0,0}(r,\vartheta,\varphi) = C_{1,0,0}\, e^{-\frac{Zr}{a_0}} \qquad a_0 = \text{ Bohr radius}$$

$$= \frac{\hbar^2}{k_{EM} m_e e^2} = 0.0529\ \mu\text{m}$$

Normalize:

$$1 = \int_{\substack{all\\space}} dV \left|\psi_{1,0,0}(r,\vartheta,\varphi)\right|^2 = \int_0^{\infty} dr\, r^2 \int_0^{\pi} d\vartheta \sin\vartheta \int_0^{2\pi} d\varphi \left|\psi_{1,0,0}(r,\vartheta,\varphi)\right|^2$$

2 $\quad 2\pi$

7. Ground state and beyond

Ground state and beyond

$$\text{So } C_{1,0,0} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \quad \text{and} \quad \psi_{1,0,0}(r,\vartheta,\varphi) = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr}{a_0}}$$

$$\textbf{Similarly} \quad \psi_{2,0,0}(r,\vartheta,\varphi) = C_{2,0,0}\left(2-\frac{Zr}{a_0}\right) e^{-\frac{Zr}{2a_0}}$$

$$\textbf{and} \quad \psi_{2,1,0}(r,\vartheta,\varphi) = C_{2,1,0}\frac{Zr}{a_0}\, e^{-\frac{Zr}{2a_0}}\cos\vartheta$$

$$\psi_{2,1,\pm1}(r,\vartheta,\varphi) = C_{2,1,\pm1}\frac{Zr}{a_0}\, e^{-\frac{Zr}{2a_0}}\sin\vartheta\, e^{\pm i\varphi}$$

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8. Radial probabilities

Radial probabilities ($r^2|R(r)|^2$)

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9. More radial probabilities

More radial probabilities

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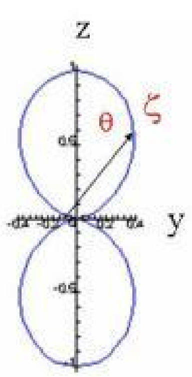
10. Angular dependence

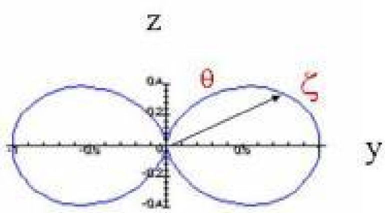
Angular dependence $2p_0$



Plot of $cos^2\theta$ shown in Y-Z plane for m_l=0. Rotate around z-axis (barbell shape). Where ζ for curve is large the probability for that θ is large.

11. Angular dependence cont'd

Angular dependence $2p_{\pm1}$



Plot of $sin^2\theta$ shown in Y-Z plane for $m_l=\pm1$. Rotate around z-axis (donut shape). Where ζ for curve is large the probability for that θ is large.

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12. Electron magnetic moment

Electron magnetic moment

electron's motion causes $\vec{\mu} = \frac{q}{2m_q}\vec{L}$ $\left(\vec{B} \propto \vec{r} \times \vec{j} \propto q\vec{r} \times \vec{v} \propto \frac{q}{m_q}\vec{L}\right)$

$\rightarrow \vec{\mu} = -\frac{e}{2m_e}\vec{L}$ for orbitting electron

QM rules $\rightarrow |\vec{\mu}| = \frac{e}{2m_e}\sqrt{l(l+1)}\hbar = \sqrt{l(l+1)}\mu_B$

Bohr magneton: $\mu_B = \frac{e\hbar}{2m_e} = 9.27 \times 10^{-24}$ J / Tesla

$= 5.79 \times 10^{-5}$ eV / T

and $\mu_z = -\frac{e}{2m_e} m_l \hbar = -m_l \mu_B$

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13. Magnetic moment problems

Magnetic moment problems

Fine structure of H spectrum indicates some l dependent departure from degeneracy. Circulating e will have a dipole interaction with magnetic field (from motion around electric Field).

$-\vec{\mu} \bullet \vec{B}$ is the energy of a magnetic dipole in B field and it alters $E_{n(l)}$ by a small amount. This does not agree with measurements.

The Zeeman effect involves the same small energy
$\rightarrow$ anomalous results

14. Electron spin

Electron spin

- Pauli - Goudsmit and Uhlenbeck - electron has intrinsic spin

$$\left|\vec{S}\right| = \sqrt{s(s+1)}\hbar \text{ with } s = \frac{1}{2} \text{ and } m_s = \pm\frac{1}{2}$$

s = 1/2 half integer spin
2s+1=2 multiplicity

e spin gets $\mu_z^{(s)} = -g_s m_s \mu_B$ with g_s gyromagnetic ratio
$g_s = 2.00232$

$\mu^{(s)}$ can interact with B field also
need extra label for $\psi_{n,l,ml,ms}$ and extra states