Physics 123 - April 22, 2013

Time Independent Schödinger equation (ld, nourelativistic)

$$
-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \psi(x)}{\partial x^{2}}+V(x) \psi(x)=E \psi(x)
$$

$|\psi(x)|^{2} d v \equiv$ probability of finding particle in $d v$ $\int_{\substack{\text { all } \\ \text { Space }}}|\psi(x)|^{2} d v=1 \quad$ Particle is Someplace

Sub in for $V$, solve for $\psi$ and $E$

H atom

$$
\rightarrow \vec{r} \rightarrow e^{-} \quad V(r)=\frac{1}{4 \pi \epsilon_{0}} \frac{|e|^{2}}{r^{2}}
$$

Shr. equ in $3 d$

$$
\underbrace{3 d}-\frac{\hbar^{2}}{2 M} \nabla^{2} \psi+V \psi=E \psi
$$

plug in $V$ and solve need to was spherical polar coordinates

## Spherical Coordinates

$$
\begin{aligned}
& x=r \sin \theta \cos \varphi \\
& y=r \sin \theta \sin \varphi \\
& z=r \cos \theta \\
& \frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}+\frac{\partial^{2} f}{\partial z^{2}}= \\
&=\frac{1}{r^{2}} \frac{\partial}{\partial r}\left(r^{2} \frac{\partial f}{\partial r}\right)+\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial f}{\partial \theta}\right)+\frac{1}{r^{2} \sin ^{2} \theta} \frac{\partial^{2} f}{\partial \varphi^{2}}
\end{aligned}
$$

$$
\begin{array}{ll} 
& \rightarrow \psi(r, \theta, \varphi) \\
V(r)=-\frac{1}{4 \pi \epsilon_{0}} \frac{|e|^{2}}{r^{2}} \\
-\frac{\hbar^{2}}{2 m}\left[\frac{1}{r^{2}} \frac{\partial}{\partial r} r^{2} \frac{\partial \psi}{\partial r}+\frac{1}{r^{2} \sin ^{2} \theta} \frac{\partial^{2} \psi}{\partial \varphi^{2}}+\frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial \psi}{\partial \theta}\right]-\frac{1}{4 \pi t_{0}} \frac{|e|^{2}}{r^{2}} \psi=E \psi
\end{array}
$$

Now Solve

Can be solved exactly...


$$
\psi(r, \theta, \varphi) \rightarrow \psi(R) \psi(\Theta) \psi(\Phi)
$$

can separate Sch. equation into egos for $\psi(R), \psi \Theta, \psi(\bar{D})+$ Solve "Energy " or "principle" quantum \# $n=1,2,3 \ldots$
"orbital" quantum $4=\quad l=0,1, \cdots n-1$
Table 7.1 spae Hydrogen Atom Wave Functions $-l,-\mid \ell-11, \cdots 0,1, \cdots, l-1,1$



$$
\begin{array}{llll} 
& \Psi_{n, l, m_{l}}(\mathbf{r})=R_{n, l}(r) Y_{l, m_{l}}(\theta, \phi) \\
n=1 & l=0 & m_{l}=0 & \psi_{100}=\frac{2}{\sqrt{r_{0}^{3}}} e^{-r / r_{0}} \sqrt{\frac{1}{4 \pi}} \\
n=2 & l=0 & m_{l}=0 & \psi_{200}=\frac{1}{\sqrt{2 r_{0}^{3}}}\left(1-\frac{r}{2 r_{0}}\right) e^{-r / 2 r_{0}} \sqrt{\frac{1}{4 \pi}} \\
n=2 & l=1 & m_{l}=+1 & \psi_{211}=\frac{1}{2 \sqrt{6 r_{0}^{3}}}\left(\frac{r}{r_{0}}\right) e^{-r / 2 r_{0}} \sqrt{\frac{3}{8 \pi}} \sin \theta e^{i \varphi} \\
n=2 & l=1 & m_{l}=0 & \psi_{210}=\frac{1}{2 \sqrt{6 r_{0}^{3}}}\left(\frac{r}{r_{0}}\right) e^{-r / 2 r_{0}} \sqrt{\frac{3}{4 \pi}} \cos \theta \\
n=2 & l=1 & m_{l}=-1 & \psi_{21-1}=\frac{1}{2 \sqrt{6 r_{0}^{3}}}\left(\frac{r}{r_{0}}\right) e^{-r / 2 r_{0}} \sqrt{\frac{3}{8 \pi}} \sin \theta e^{-i \varphi p}
\end{array}
$$

Probability distributions for several allowed atomic states for the 1-electron atom

Increasing n adds new radial layers, l=0 give spherical symmetry, I not 0 brings in angular dependence


Only discrete energies and spatial sites allowed for the election to occupy $\rightarrow$ orbital

figure from h Hpp:/len.wik:pedia.org/wik:/File: Hydrogen_Density_Pots. pry


Hydrogen $z=1$
Helvin $z=2$
Lith.in $z=3$

$$
z=120
$$

O $Z$ protons
0 \& $(A-Z)$ neutions 0

Basic Stinctur of atom

as $Z$ increases $\rightarrow$ elections increase个
\#protons in nucleus
Hows do these elections populate the available orbitals?
To Answer this we Need to investigate

STern-Gerlach experiment - 1922
$\rightarrow$ Discovery that electrons have Spin


Diagram from Wikipedia
"If this nonsense from Bohr will Prove to be right we will quit physics." (Stem vowed in 1913 ) asquoted in Phys. Today $\operatorname{Dec} 03$

Walther Gerlach from phys Today antizle (Dec. 03)

General Quant. Mech. result regarding force on magnetic dipole in a non-uniform magnetic field

$$
\vec{F}_{z}=\frac{\partial B_{z}}{\partial z}\left|\vec{\mu}_{z}\right|=\frac{\partial B_{z}}{\partial z} m
$$

Stern-Gerlach experiment
e- beam in l=1 state
has $m=1,0,-1$ components


General Quant. Mech. result regarding force on magnetic dipole in a non-uniform magnetic field

$$
\vec{F}_{z}=\frac{\partial B_{z}}{\partial z}\left|\vec{\mu}_{z}\right|=\frac{\partial B_{z}}{\partial z} m
$$

Stern-Gerlach experiment
e- beam in l=0 state
Has m=0-component only


SURPRISE! ... fundamental particle have an intrinsic magnetic moment. Call it spin.

$$
\vec{F}_{z}=\frac{\partial B_{z}}{\partial z}\left|\vec{\mu}_{z}\right|=\frac{\partial B_{z}}{\partial z} m
$$

Stern-Gerlach experiment
e - beam in $\mathrm{l}=0$ state
Has $m=0$ component only


Particles hove intrinsic Spin


Spin is quantized

$$
0,1 / 2,1,3 / 2,2,5 / 2
$$

## Intrinsic spin - two varieties

## Huge effect on

multi-electron
atoms
Fermions = half integral spin, s/ach as $1 / 2,3 / 2,5 / 2, \ldots, 73 / 2 \ldots$ protons, neutrons, electrons are all fermions ( $s=1 / 2$ ) no two fermions can occupy the same exact quantum state

Bosons = integral spin, such as $0,1,2 \ldots$
photons ( $s=1$ ) and pions ( $s=0$ ) are examples of bosons bosons can occupy the same exact quantum state

## Rules for Filling of state for multi-electron atom

 $n, 1, m_{1,} m_{s}$Spectroscopic notation - s: l=0, p: l=1, d: l=2, f: l=3, ...
$>$ No two electrons in same state (Pauli exclusion)
$>$ Electrons go into the state with the lowest possible energy (Aufbau)
$>$ Within a sublevel, electrons will have their spin unpaired as much as possible (due to spin-spin interaction contribution to energy)


## TABLE 39-1 Quantum Numbers for an Electron

| Name | Symbol | Possible Values |
| :--- | :--- | :--- |
| Principal | $n$ | $1,2,3, \cdots, \infty$. |
| Orbital | $\ell$ | For a given $n: \ell$ can be $0,1,2, \cdots, n-1$. |
| Magnetic | $m_{\ell}$ | For given $n$ and $\ell: m_{\ell}$ can be $\ell, \ell-1, \cdots, 0, \cdots,-\ell$. |
| Spin | $m_{s}$ | For each set of $n, \ell$, and $m_{\ell}: m_{s}$ can be $+\frac{1}{2}$ or $-\frac{1}{2}$. |


P.A.M. Dirac - on the development of quantwn Mechanics "The underlying laws necessary for the mathematical theory of a large part of physics and the whole of chemisting are thus completely knows.



Check out
http:www.chemicool.com
Interactive periodic chart







$i 0_{\text {gich }}^{i-2}$


そ $e_{e}^{-} \bar{z}$

Covalent bond

