# ECE 495N

# Fundamentals of Nanoelectronics

## Fall 2008

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**Purdue University**

**Lecture: 11**
**Title: Valence Electrons and Charging Energy**
**Date: September 14, 2008**

**Video Lectures posted at:**
**https://www.nanohub.org/resources/5346/**

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PURDUE UNIVERSITY

# Valence Electrons and Charging Energy

## Lecture 11

Sept. 14, 2008

$$E\Phi = \left(-\frac{\hbar^2}{2m}\nabla^2 + \underbrace{U(r)}_{\text{negative}} + \underbrace{U_e(r)}_{\text{positive}}\right)\Phi$$

potential that the electron feels due to nucleus

electron-electron interaction

$$\Phi(\vec{r}) = \frac{g(r)}{r} Y_\ell^m(\theta, \phi)$$

$m$: $-\ell, \ldots, +\ell$

$\ell$: $0, 1, \ldots$

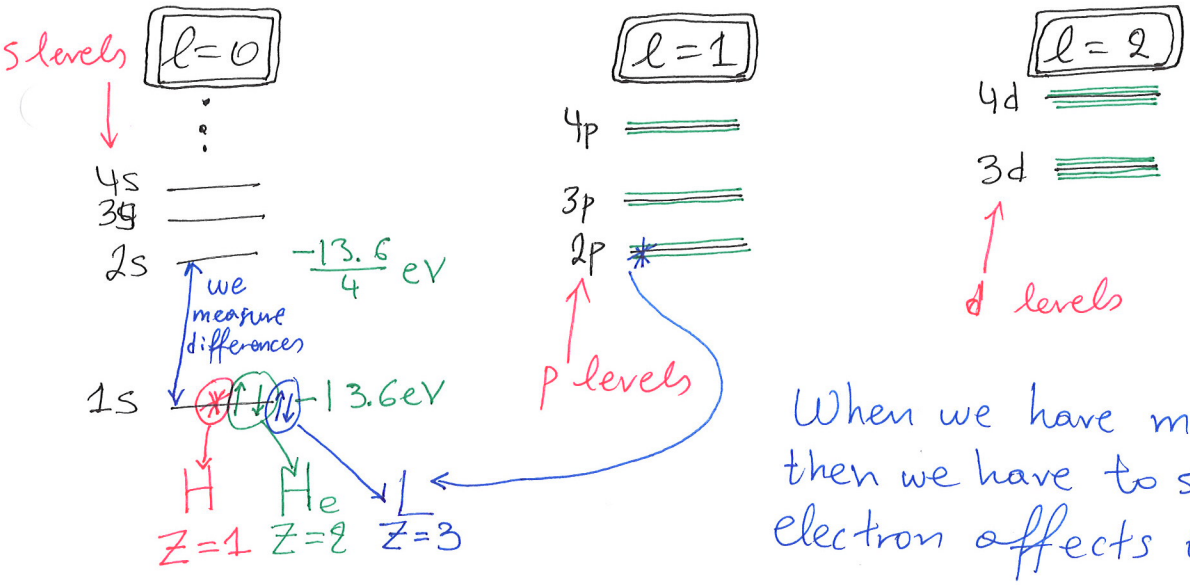
$$Eg = \left(\underbrace{-\frac{\hbar^2}{2m}\frac{d}{dr^2}}_{\text{triadiagonal matrix (due to nucleus)}} + \underbrace{\frac{\ell(\ell+1)\hbar^2}{2mr^2}}_{\text{diagonal matrix (when } \ell \neq 0)} + U(r)\right) g$$

$e$ $\quad +Z$

$$U = -\frac{Zq^2}{4\pi\epsilon_0 r}$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

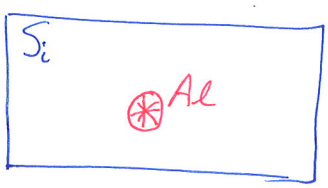
not seperable in cartersian

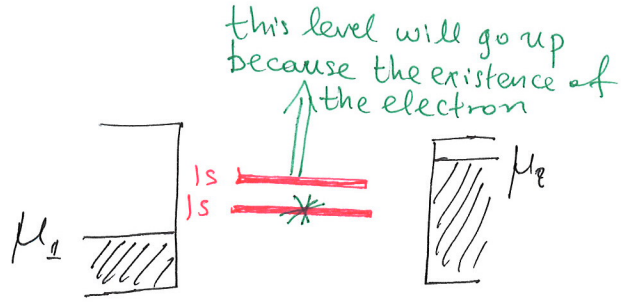


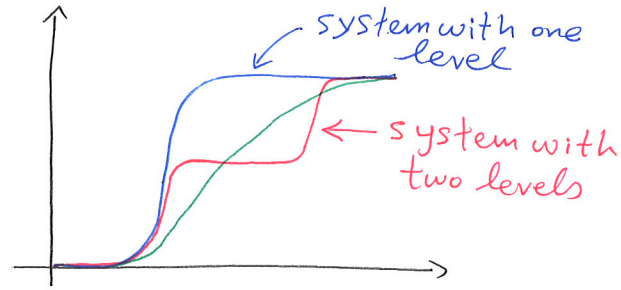

In addition all the levels come in pairs

When we have more electrons then we have to see how each electron affects the others.

All the action of electrons is occured in the valence electrons. These are outmost level.






<u>Self interaction</u>: each electron does not feel something from itself only from the others. That's the reason that only one level floats up and not both of them. This is part that makes very hard to add it up to the S.E. and to solve it.

The interaction is taking into account by

$$\underset{10^{-6}}{\overset{10^{-5}}{U_0}}\,(\underset{10^{6}\pm 1}{\overset{2}{N}}-N_0)$$