Qualitative understanding of many-electron atoms

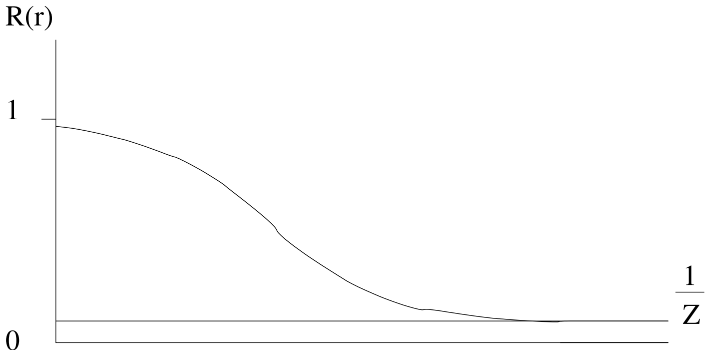
1. centr. field $\Upsilon(r)$ “close“ to $+Ze$ nucleus

$$V(r) = -\frac{Ze^2}{r}$$

the ratio $R(r)$

$$R(r) = \frac{\Upsilon(r)}{V(r)} = \frac{\Upsilon(r)}{-\frac{Ze^2}{r}}$$

is such that close to nucleus, $R(r \to 0) \to 1 - \frac{5}{16Z} \approx 1$ while for large r $R(r \to \infty) \to \frac{1}{Z}$



$$(1s)^2(2s)^2(2p)^6 \to Ne$$

$(1s)^2(2s)^2(2p)^6 \to Ne$

$(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^{10} \to Ni$ But this does not work

---

E_n : $E_{n,l} = E_n$ in hydrogen-like case

but in $\Upsilon(r)$

is such that

$E_{n,l_1} < E_{n,l_2}$ if $l_1 < l_2$

see the difference Boron - Beryllium in the table

Radial equation

$$T_r + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + \Upsilon(r)$$

with increasing ℓ the wavefunction is pushed outside (to large r)

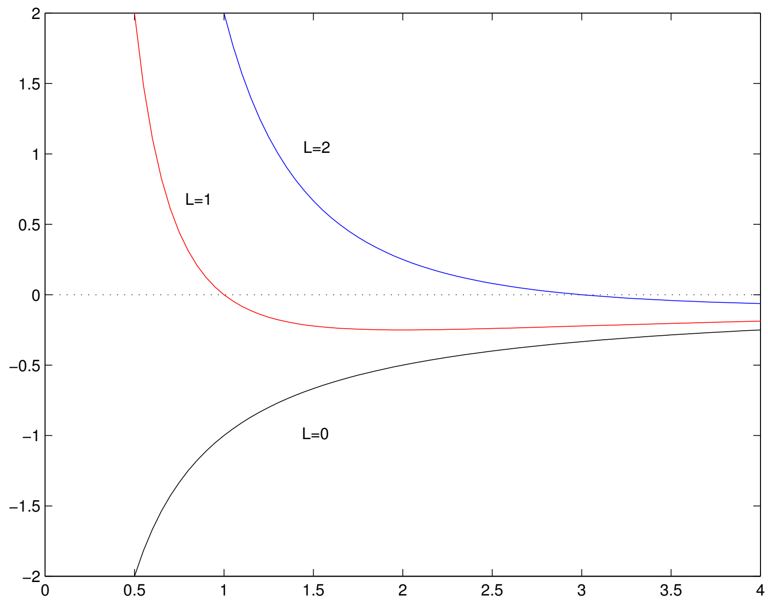
for small ℓ (especially $\ell = 0$) it is easy for the electrons to see the region where the potential is not screened

for $\ell = 0$ the electrons can ”see” the nucleus

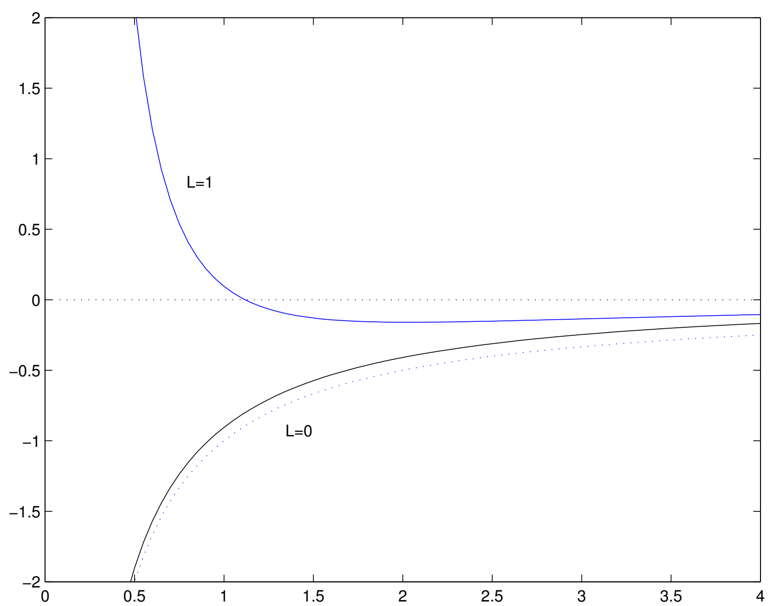
Thus effectively

$$E_{n,l} = E_n + f(l) * \Delta E$$

$$f(l) \equiv f(l,n) \geq 0$$



The above picture is the Coulomb potential



The above picture is the Hartree potential, represented by an exponentielly screened function (The Coulomb potential is the dotted line)