Coulombian potential energy: Hydrogen-like ions (`Hydrog.m`)

I. CONFINED STATE ENERGIES

For an hydrogen-like ion of atomic number Z, the potential energy of the electron is:

$$\mathcal{E}_p(x) = -\frac{A}{x} + \frac{B}{2x^2} \quad \text{with} \quad A = q_e^2 = \frac{e^2}{4\pi\varepsilon_0} \quad \text{and} \quad B = \frac{\ell(\ell+1)\hbar^2}{m_e}$$

x being the distance between the electron and the nucleus and ℓ the quantum number of the orbital angular momentum. Potential energy can be written using the depth of the well $\mathcal{E}_{p,0}$, the corresponding distance x_0, the rydberg Ry, and the Bohr radius a_B. Indeed:

$$\mathcal{E}_{p,0} = \frac{Z^2 Ry}{\ell(\ell+1)} = \frac{1}{\ell(\ell+1)} \frac{m_e}{2} \left(\frac{Zq_e^2}{\hbar}\right)^2 = \frac{A^2}{2B}$$

and

$$x_0 = \ell(\ell+1)\frac{a_B}{Z} = \frac{\ell(\ell+1)\hbar^2}{m_e Z q_e^2} = \frac{B}{A} \quad \text{so that} \quad A = 2x_0\mathcal{E}_{p,0} \quad \text{and} \quad B = 2x_0^2\mathcal{E}_{p,0}$$

Finally:

$$\mathcal{E}_p(x) = 2\mathcal{E}_{p,0}\left(-\frac{x_0}{x} + \frac{x_0^2}{2x^2}\right)$$

For hydrogen, $Z = 1$ and $\ell = 1$. The following commands:

```
Z=1; l=1; m=1; [sys,E]=Hydrog(Z,l,m);
```

returns the Figure 1a. On Table I, the values of the confined state energy $\mathcal{E}_n^{(si)}$ obtained by simulation are compared to that theoretically calculated with $\mathcal{E}_n^{(th)} = -Z^2 Ry/n^2$.

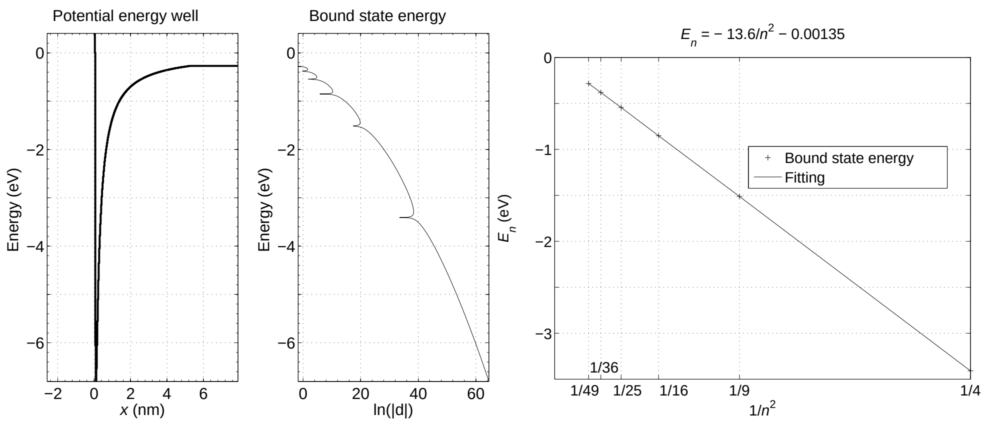
$\ell = 1$			$\ell = 2$		
n	$\mathcal{E}_n^{(si)}$ (eV)	$\mathcal{E}_n^{(th)}$ (eV)	n	$\mathcal{E}_n^{(si)}$ (eV)	$\mathcal{E}_n^{(th)}$ (eV)
2	-3.409	-3.402	8	-0.212	-0.213
3	-1.512	-1.512	9	-0.168	-0.168
4	-0.852	-0.850	10	-0.136	-0.136
5	-0.544	-0.544	11	-0.112	-0.112
6	-0.381	-0.378	12	-0.094	-0.094
7	-0.283	-0.278			

TAB. I – *Some confined state energies of an electron in Hydrogen*

Since $\ell = 1$, the first value for n is 2. Indeed, the value $\mathcal{E}_1 \approx -13.6\,\mathrm{eV}$ cannot be reached since it is lower than $-\mathcal{E}_{p,0}$. However, it can be extrapolated by plotting $\mathcal{E}_n$ versus $1/n^2$:

```
En=-[3.409;1.512;0.852;0.544;0.381;0.283]; n=[2;3;4;5;6;7];
plot(n.^(-2),En,'r+',n.^(-2),En,'b');grid on;
set(gca,'xtick',[1/49,1/36,1/25,1/16,1/9,1/4],...
'xticklabel',{'1/49','1/36','1/25','1/16','1/9','1/4'});
xlabel('1/n^2'); ylabel('En (eV)');
```

A linear interpolation gives the equation $\mathcal{E}_n = -13.6/n^2 + 0.00135$ (Fig. 1b), which then provides $\mathcal{E}_1 = -13.6\,\mathrm{eV}$.



a) *b)*

FIG. 1 – *a) Confined state energies of an electron in Hydrogen* *b)* $\mathcal{E}_n$ *vs.* $1/n^2$

With $\ell = 2$, `Hydrog(1,2,1);`, one retrieves the value of the first states ($n = 2$ to 7) and the results of the last column of the Table ($n = 8$, 9, 10, 11, and 12). They are in agreement with the theoretical ones.

Note that `Hydrog.m` does not consider $\ell = 0$ because the limit $x \to 0$ tends to introduce numerical errors in the matrix method. Schrödinger equation must be solved by `Schrodinger.m`.

Obviously, muonic and positronic atoms are obtained by modifying m; furthermore Ry must thus be multiplied by μ/m_e and a_B by m_e/μ.

1. *Probability density*

Figure 2 shows the probability density ρ_p for the four first confined states; it has been obtained with:

```
Ry = 13.6058; aB = 0.0529177; l=1; Z=1;
Ep0 = Z^2*Ry/(l*(l+1)); x0 = l*(l+1)*aB/Z;
x=linspace(x0/4,50*x0,200);
Epc=2*Ep0.*(-(x0./x)+(x0^2./(2.*x.^2)));
[En,rho_n]=Schrodinger(min(x),max(x),Epc,1,4);
```

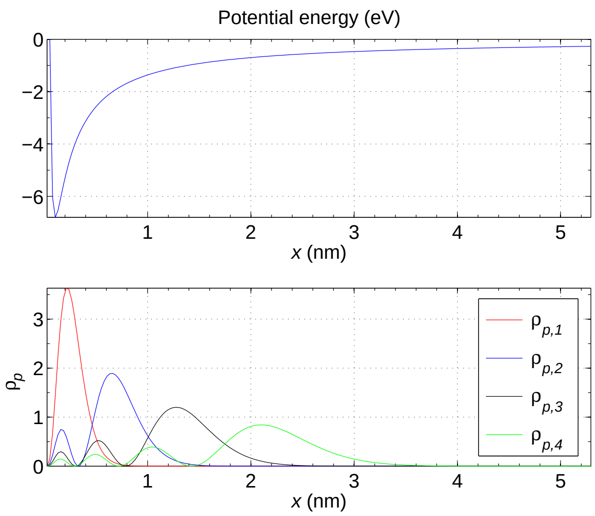


FIG. 2 – *Probability density for the four first levels of hydrogen* ($\ell = 1$)

For the hydrogen-like ion He^+ ($Z = 2$), the results given (not shown) by `Hydrog(2,2,1)` match well with the theoretical relation $-4Ry/n^2$ ($n \geq 2$).