Prof. Dr. Ibraheem Nasser Phys 551, T-132 15 February, 2012
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KING FAHD UNIVERSITY of PETROLIUM and MINERALS
Physics Department
Atomic and Molecular Physics (Phys-551)
Spring 2014

Issued: 4-2-2014	**Assignment # 2**	Due date 9-2-2014

Use MATHEMATICA and atomic units

A- Application of Virial theorem.

For the Schrödinger equation:

$$\hat{H}\psi = \left(\hat{T} + \hat{V}\right)\psi = E\psi \quad \Rightarrow \quad E = \left\langle \hat{H} \right\rangle = \left\langle \hat{T} \right\rangle + \left\langle \hat{V} \right\rangle$$

the Virial theorem state that:

$$\left\langle \hat{V} \right\rangle = \frac{2E}{n+2}, \qquad \left\langle \hat{T} \right\rangle = \frac{nE}{n+2}$$

n is the degree of the homogeneous potential, for example $V(r) \propto r^n$.

Examples:

1- For the one dimensional harmonic oscillator, $V = \frac{1}{2}kx^2 \Rightarrow n = 2$, and

$$\left\langle \hat{T} \right\rangle = \left\langle \hat{V} \right\rangle = \frac{2E}{2+2} = \frac{1}{2}E = \frac{1}{2}\hbar\omega(n + \frac{1}{2}), \qquad n = 0,1,2,\cdots$$

2- For the hydrogen atom, $V = \frac{k}{r} \quad \Rightarrow \quad n = -1, \quad E = -\frac{1}{2n^2} = -0.5 \quad \text{au}$, and

$$\left\langle \hat{V} \right\rangle = 2E = -\frac{1}{n^2} = -1.0 \text{ au}, \qquad \left\langle \hat{T} \right\rangle = -E = \frac{1}{2n^2} = 0.5 \text{ au}, \qquad \left\langle \hat{T} \right\rangle = -\frac{1}{2}\left\langle \hat{V} \right\rangle$$

Home work: Write a program to:

1- Determine the average kinetic and potential energy for the electron in the ls, 2s, 2p, and 3p states by using the **exact hydrogenic orbitals**.
2- Calculate the average kinetic and potential energy for the electron in the ls, 2s, 2p, and 3p states by using approximate orbitals given as Slater-type orbitals* (STO) with screening parameters $\zeta_{1s} = 1, \zeta_{2s} = 0.5, \zeta_{2p} = 0.5$ and $\zeta_{3p} = \frac{1}{3}$. How well is the virial theorem fulfilled for the approximate orbitals?
3- Plot the wavefunctions in both cases.

*Slater type orbital, STO, is defied as:

$$\psi_{n\ell m}(r,\theta,\varphi) = N_{n\ell} r^{n-1} e^{-\zeta_{n\ell} r} Y_{\ell m}(\theta,\varphi)$$

where $\zeta_{n\ell}$ is the orbital exponent, $Y_{\ell m}(\theta,\varphi)$ the normalized spherical harmonics and $N_{n\ell}$ normalization constant,

$$N_{n\ell} = \frac{\left(2\zeta_{n\ell}\right)^{n+\frac{1}{2}}}{\left[(2n)!\right]^{\frac{1}{2}}}$$

B- Use the linear variational method to do the following (Use atomic units):

1- Calculate the eigenvalues of 1s, 2s and 3s of the Hydrogen-like atoms by constructing 3×3 matrix.

2- Calculate the first order correction due the perturbation $H' = \dfrac{e^{-r}}{r}$