PHYS 4390 Quantum Mechanics II

Homework Assignment 05

Due date: February 21, 2019

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Mandatory problems: *ALL!* I MAKE THIS HOMEWORK SET LIKE A TEAM PROJECT. YOU CAN FORM TWO TEAMS (A TEAM OF THREE) AND EACH TEAM SUBMITS ONE SET OF SOLUTIONS FOR ALL THE PROBLEMS.

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P #	1	2	3	4	5	Score
Score	/	/	/	/	/	/100

Prob 1 Using the completeness relation for the energy eigenstates for unperturbed Hydrogen atom (without any of the corrections) show that

$$\begin{aligned}
& \langle n_1, l_1, m_1|_1 \langle n_2, l_2, m_2|_2 \frac{1}{|\vec{r}_1 - \vec{r}_2|} |n_1', l_1', m_1'\rangle_1 |n_2', l_2', m_2'\rangle_2 \\
= & \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \Lambda(l) \Omega_1(l,m) \Omega_2(l,m)
\end{aligned}$$

where

$$\begin{aligned}
\Lambda(l) = & \int_0^\infty R^*_{n_1 l_1}(r_1) R_{n_1' l_1'}(r_1) r_1^2 dr_1 \left\{ \int_0^{r_1} \frac{r_2^{l+2}}{r_1^{l+1}} R^*_{n_2 l_2}(r_2) R_{n_2' l_2'}(r_2) dr_2 \right. \\
& \left. + \int_{r_1}^\infty \frac{r_1^l}{r_2^{l-1}} R^*_{n_2 l_2}(r_2) R_{n_2' l_2'}(r_2) dr_2 \right\} \\
\Omega_1(l,m) = & \int_0^\pi \int_0^{2\pi} \sin(\theta_1) d\theta_1 d\varphi_1 Y^*_{l_1 m_1}(\theta_1,\varphi_1) Y_{l_1' m_1'}(\theta_1,\varphi_1) Y_{lm}(\theta_1,\varphi_1) \\
\Omega_2(l,m) = & \int_0^\pi \int_0^{2\pi} \sin(\theta_2) d\theta_2 d\varphi_2 Y^*_{lm}(\theta_2,\varphi_2) Y_{l_2' m_2'}(\theta_2,\varphi_2) Y^*_{l_2 m_2}(\theta_2,\varphi_2)
\end{aligned}$$

Hint: Refer to the property and relationship of the Legendre Polynomials and Spherical Harmonics in PHYS 3160.

Prob 2 We have shown in class that the energy contribution due to electron-electron interaction in a Helium atom for the first excited state is given by

$$E^{(1)}_{n\pm} = \Gamma \pm \Pi,$$

where

$$\begin{aligned}
\Gamma = & \frac{e^2}{4\pi\epsilon_0} \langle 2, l', m'|_2 \langle 1,0,0|_1 \frac{1}{|\vec{r}_1 - \vec{r}_2|} |1,0,0\rangle_1 |2, l', m'\rangle_2 \\
= & \frac{e^2}{4\pi\epsilon_0} \langle 2, l', m'|_1 \langle 1,0,0|_2 \frac{1}{|\vec{r}_1 - \vec{r}_2|} |1,0,0\rangle_2 |2, l', m'\rangle_1 \\
\Pi = & \frac{e^2}{4\pi\epsilon_0} \langle 2, l', m'|_2 \langle 1,0,0|_1 \frac{1}{|\vec{r}_1 - \vec{r}_2|} |1,0,0\rangle_2 |2, l', m'\rangle_1
\end{aligned}$$

Applying the relation you derived in problem 1, for $l' = 1, m = 0$ show that

(a)

$$\begin{aligned}
\Gamma = & \frac{e^2}{4\pi\epsilon_0} \int_0^\infty |R_{10}(r_1)|^2 r_1^2 dr_1 \left\{ \frac{1}{r_1^2} \int_0^{r_1} |R_{21}(r_2)|^2 r_2^3 dr_2 + r_1 \int_{r_1}^\infty |R_{21}(r_2)|^2 dr_2 \right\} \\
\Pi = & \frac{e^2}{4\pi\epsilon_0} \int_0^\infty R^*_{10}(r_1) R_{21}(r_1) r_1^2 dr_1 \left\{ \frac{1}{r_1^2} \int_0^{r_1} R^*_{21}(r_2) R_{10}(r_2) r_2^3 dr_2 \right. \\
& \left. + r_1 \int_{r_1}^\infty R^*_{21}(r_2) R_{10}(r_2) dr_2 \right\}.
\end{aligned}$$

(b) The expression for Γ describes purely classical electrostatic energy of two interacting electrons.

Prob 3 For a Helium atom when one of the electron is in the state $1s$ and the other in the $2s$, we have found

$$\begin{aligned}
\Gamma = & \frac{e^2}{4\pi\epsilon_0} \int_0^\infty |R_{10}(r_1)|^2 r_1^2 dr_1 \left\{ \frac{1}{r_1} \int_0^{r_1} |R_{20}(r_2)|^2 r_2^2 dr_2 + \int_{r_1}^\infty |R_{20}(r_2)|^2 r_2 dr_2 \right\} \\
\Pi = & \frac{e^2}{4\pi\epsilon_0} \int_0^\infty R^*_{10}(r_1) R_{20}(r_1) r_1^2 dr_1 \left\{ \frac{1}{r_1} \int_0^{r_1} R^*_{20}(r_2) R_{10}(r_2) r_2^2 dr_2 \right. \\
& \left. + \int_{r_1}^\infty R^*_{20}(r_2) R_{10}(r_2) r_2 dr_2 \right\}
\end{aligned}$$

and when one electron in the state $1s$ and the other in $2p$,

$$\Gamma' = \frac{e^2}{4\pi\epsilon_0}\int_0^\infty |R_{10}(r_1)|^2 r_1^2 dr_1 \left\{\frac{1}{r_1^2}\int_0^{r_1} |R_{21}(r_2)|^2 r_2^3 dr_2 + r_1 \int_{r_1}^\infty |R_{21}(r_2)|^2 dr_2\right\}$$

$$\Pi' = \frac{e^2}{4\pi\epsilon_0}\int_0^\infty R_{10}^*(r_1) R_{21}(r_1) r_1^2 dr_1 \left\{\frac{1}{r_1^2}\int_0^{r_1} R_{21}^*(r_2) R_{10}(r_2) r_2^3 dr_2 \right.$$
$$\left. + r_1 \int_{r_1}^\infty R_{21}^*(r_2) R_{10}(r_2) dr_2\right\}.$$

(a) Using the appropriate radial part of the wave functions and computers (I suggest Mathematica) find the numerical values for the energy Γ, Π, Γ', and Π'.

(b) Using the numerical values you determined find the energy contributions

$$E_1^{(1)} = \Gamma + \Pi, E_2^{(1)} = \Gamma - \Pi, E_3^{(1)} = \Gamma' + \Pi', E_4^{(1)} = \Gamma' - \Pi'$$

(c) The values given in the textbook are

$$E_{1,2}^{(1)} = 11.4eV \pm 1.2eV, E_{3,4}^{(1)} = E_{1s,2p}^{(1)} = 13.2eV \pm 0.9eV.$$

does your numerical results agree with these values? If not, identify where I/you went wrong.

(d) By providing a convincing physical argument identify which energy values $(E_1^{(1)}, E_2^{(1)}, E_3^{(1)}, E_4^{(1)})$ belong to the singlet or triplet states.

Prob 4 Townsend *Problems 12.3, 12.4, and 12.6*

Prob 5 Applying *Gram-Schmidt orthogonalization method* we have shown that the trial state vector for the first excited state is given by

$$|\psi_1\rangle = \frac{|\psi\rangle - \langle E_0 |\psi\rangle |E_0\rangle}{\sqrt{2\left(1 - |\langle E_0 |\psi\rangle|^2\right)}},$$

where $|\psi\rangle$ *an arbitrary square integrable trial state vector,* $|\psi\rangle$.

(a) Following a similar procedure determine the trial state vector for the second excited state.

(b) Using this trial state vector, $|\psi_1\rangle$, find the energy values for the first excited state. *Use of computers may be helpful...*