Química Física I
Grado en Química

UNIVERSIDAD DE MURCIA

Lesson: APPROXIMATE METHODS IN QUANTUM MECHANICS

PROBLEM SHEET: QUESTIONS

1. (♦♦♢) Use the $\psi(r) = e^{-cr}$ function to describe the ground state of the hydrogen atom. Find the value of c which minimizes the variational integral.

2. (♦♦♢) Use the $\psi(r) = e^{-cr^2/a_0^2}$ function to describe the ground state of the hydrogen atom. Find the value of c which minimizes the variational integral and the error with respct to the accurate energy.

3. (♦♦♦) Use the following variational function

$$\phi(x) = c_1 x^2(l-x) + c_2 x(l-x)^2$$

to describe a particle in a one-dimensional box. Calculate the variational approximations to the energies of the first two levels, their corresponding errors with respect to the accurate energies and their c_1/c_2 ratios.

4. (♦♦♢) Consider the following one-dimensional model which potential energy is given by

$$\begin{cases} +\infty & x < 0 \\ 0 & 0 < x < \frac{l}{4} \\ V_0 & \frac{l}{4} < x < \frac{3l}{4} \\ 0 & \frac{3l}{4} < x < l \\ +\infty & x > l \end{cases}$$

where $V_0 = \hbar^2/ml^2$. Apply the perturbation theory considering the $V_0 = 0$ model as zero order approximation. Calculate the first order corrections to the energy of the first two levels.

Dificulty level: (♦♢♢) Easy, (♦♦♢) Normal, (♦♦♦) To think a bit.

PROBLEM SHEET: SOLUTIONS

Question 1 $\Rightarrow$ $c = \frac{Z}{a_0}$

Question 2 $\Rightarrow$ $c = \frac{8}{9\pi}$, 15.1%

Question 3 $\Rightarrow$ $W_1 = \frac{5\hbar^2}{ml^2}$, $W_2 = \frac{21\hbar^2}{ml^2}$, 1.32%, 6.38%, $c_1 = c_2$ y $c_2 = -c_1$