Química Física I
Grado en Química

UNIVERSIDAD DE MURCIA

Lesson: INTRODUCTION TO QUANTUM CHEMISTRY

PROBLEM SHEET: QUESTIONS

1. (♦◇◇) Let Ψ_1 and Ψ_2 be two degenerate solutions of the Schrödinger's equation. Verify that any linear combination $\Psi = a\Psi_1 + b\Psi_2$ (being a and b two scalars) is also solution of the Schrödinger's equation for the same system and with same value of the energy.

2. (♦◇◇) Assuming that $\hat{D} = \frac{d}{dx}$ prove that $(\hat{D} + \hat{x})(\hat{D} - \hat{x}) = \hat{D}^2 - \hat{x}^2 - 1$

3. (♦◇◇) Prove that $(\hat{A} + \hat{B})^2 = (\hat{B} + \hat{A})^2$ for any two operators. Under what conditions the identity $(\hat{A} + \hat{B})^2 = \hat{A}^2 + 2\hat{A}\hat{B} + \hat{B}^2$ is valid?

4. (♦♦◇) Which of the following functions are eigenfunctions of the $\frac{d^2}{dx^2}$ operator? (a) e^{bx} (b) $e^{ax} + e^{bx}$ (c) $a\sin x + b\cos x$, being a and b scalars. Get the corresponding eigenvalues.

5. (♦♦◇) Let us consider a particle moving in the (x, y, z) space. Evaluate the following commutators: (a) $[\hat{x}, \hat{p}_x]$ (b) $[\hat{x}, \hat{p}_y]$ (c) $[\hat{x}, \hat{p}_x^2]$ (d) $[\hat{x}, V(x, y, z)]$

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

PROBLEM SHEET: SOLUTIONS

Question 3 ⇒ $[\hat{A}, \hat{B}] = 0$

Question 4 ⇒ (a) b^2 (b) a^2 si $a = b$ (c) -1

Question 5 ⇒ (a) $i\hbar$ (b) 0 (c) $2\hbar^2 \frac{\partial}{\partial x}$ (d) 0