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Faculty of Material Sciences and Computer Science

Department of Chemistry 3 rd Year LMD SM (2025/2026)

Exercise Series No. 03

Exercise 1:

We will solve the time-independent Schrödinger equation for the hydrogen atom by seeking wave functions that depend only on r (s atomic orbitals).

Under these conditions, the Laplacian Δ is written as:

$$\Delta = \frac{1}{r2}\frac{d}{dr}(r^2\frac{d}{dr})$$

a- Show that ψ (r) =A exp (-B r) is a solution of this equation.
b- Calculate the value of the constant B. Identify this value.
c- Calculate the corresponding energy.
d- Determine the constant A

Exercice 2:

The hydrogen atom in its ground state is described by the previous wave function.

1. Verify that within a sphere of radius r=3,14 a_0, the probability of presence is 95%.

(a_0 radius of the first Bohr orbit, a_0 = 0.53 Å)

Recall: In spherical coordinates, the volume element is:

$$dV = r^2 \sin\theta dr d\theta d\emptyset$$

Given:

$a_0 = h^2\varepsilon_0/\pi me^2$

$\int_0^{\infty} r^2 e^{-\alpha r}\ dr = n!/\alpha^{n+1}$ avec n > 0 et α > 0

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