

CHEM356: PHYSICAL CHEMISTRY II
HOMEWORK SET III - DUE 18th OF APRIL, 5.00 PM
Each problem is worth 5 points, 25 pts in total.

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Problem I

- Show that \hat{L}^2 commutes with \hat{L}_x . (use spherical coordinates).
- Using cartesian coordinates, show that:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

Problem II

Imagine a He^+ ion with a single electron at $2p_z$ orbital. What is average position $\langle r \rangle$ and most probable distance from the nucleus for this electron?

Problem III

Imagine a hydrogen atom in an excited state with an electron at 2s orbital.

1. Compute the two maxima of the probability function the electron $r^2|\psi_{2s}(r)|^2$.
2. Compute the position of the radial node, at which probability of finding the electron is equal to 0.
3. Finally, compute the radius of the sphere that captures 90% probability of finding the 2s electron.

Problem IV

On example of hydrogen-like orbitals, show that the charge density of the fully occupied subshell (for instance $2p^6$) is spherically symmetrical. (In practice, show that there is no angular dependence in the sum of squares of three spherical harmonics with $l=1$).

MM: The result is somewhat intuitive, but common visualizations of p and d orbitals are often misleading.

Problem V

1. Write down the complete hamiltonian for the lithium atom. Identify respective terms.
2. Write down the Slater determinant Φ^{SSD} for the ground-state configuration of lithium atom.