

Problem 1. Consider quantum-mechanical rotations in three dimensions (aka 3D rigid rotor or particle on a sphere) corresponding to the quantum number $l = 3$. Calculate and list all values of the angle between the vector of the angular momentum and the z axis.

Problem 2. Consider an excited state of hydrogen atom with electron in the 3p orbital with $m_l=1$. Answer the following questions. You don't need to provide fully numerical answers – they can be expressed via a combination of numerical factors and physical constants, like e , \hbar , ϵ_0 , a_0 , etc

A. Write the expression for the probability density to find the electron at a given point (r, θ, ϕ) in the 3D space. (You may leave the numerical factors as they are: no need to reduce or calculate them.)

B. In which point(s) in the 3D space within the atom you are unlikely to find the electron?

C. At what distance from the nucleus you are most likely to find the electron? (If you have problems finding the answer analytically through derivative, you can try to answer this question by graphing the corresponding probability)

D. Determine the average distance of the electron from the nucleus.

E. Calculate the average potential energy of the electron in this orbital and compare it with the total energy in this state. Does the relationship $\langle V \rangle = 2E$ we derived in class for the 1s and in your HW#3 for 2p orbital still hold?

F. Calculate the angle between the vector of the orbital angular momentum of the electron and the z-axis.

G. What is the smallest quantum of energy required for this electron to leave the atom?

Problem 3. Consider a gas of iodine (I_2) molecules at standard temperature and pressure (0°C and 1 atm (101.325 kPa)). The rotational constant for molecular iodine is 0.03737 cm^{-1} , the force constant is 172 N/m. The atomic mass of iodine is 127 a.m.u. Answer the following six questions. *Show your calculations.*

A. Calculate the molecular partition function for vibrations of molecular iodine at these conditions. *Explain your assumptions.*

B. What fraction of iodine molecules on average occupy the first excited vibrational energy level at this temperature? *Explain your assumptions and support with calculations if needed.*

C. Calculate the molecular partition function for rotations of molecular iodine at these conditions. *Explain your assumptions and support with calculations if needed.*

D. What fraction of iodine molecules on average occupy the first excited rotational energy level at this temperature? *Explain your assumptions and support with calculations if needed.*

E. Calculate the contribution from rotational motion to the entropy of 1 mole of iodine molecules at these conditions. *Explain your assumptions.*

F. Calculate the molecular partition function for translational motion of iodine molecule at these conditions. *Explain your assumptions.* (Because this question is about the molecular partition function, you can treat the molecules as distinguishable.)