Problem Solving Class: Van Quark tot Biomaterie

Problem Set 8: Quantum states and transitions Hand-in on paper Thursday 16 October Hand-in digitally, email to: <u>m.t.talluri@vu.nl</u>; All documents in a single file [file: YourName-WC-Q8] All answers in English

1) Thermal population of quantum states

- a) What is the statistical probability to find a hydrogen atom in the excited 2s state, for conditions of room temperature (with respect to ground state 1s).
- b) What is the probability to find a hydrogen molecule in its v=1 vibrationally excited state (calculate for T=50 K, the typical condition for an interstellar cloud).
- c) Same for rotational excitation in the J=1 state for the hydrogen molecule (for room temperature). Calculate in this case the relative population with respect to J=0.

2) Dynamics of a two level system

Consider a "two-level system" with energy levels E_2 (upper level) and E_1 (lower level) with populations $n_2(t)$ and $n_1(t)$. A rate equation including spontaneous emission with rate A, absorption with rate Bu_v and stimulated emission with rate Bu_v can be written as follows:

$$\frac{d}{dt}n_2(t) = Bu_v n_1(t) - \left(A + Bu_v\right)n_2(t)$$

- a) Solve this differential equation for $n_2(t)$ for boundary conditions $n_1(0)=N$ and $n_2(0)=0$, where $N = n_2(t) + n_1(t)$ is the total number of atoms, independent of time.
- b) Show that at short times, defined as $(A + 2Bu_v)t \ll 1$, there is a steady growth of population in the excited state.
- c) How is the behaviour for $t \rightarrow \infty$?
- d) Show that there is a maximum population for n_2 for all times and for all intensities u_v . Consider even $u_v \rightarrow \infty$. i.e. infinitely strong intensity.

The above **should** be done analytically, including the solution to the differential equation.

You may also use Mathematica (additionally) to solve the problems. Tip: simplify the results by : "Simplify[]".

Plot $n_2(t)$ for different values of the ratio A ad Bu_v and try to find a numerical answer to the questions stated above.

3) CO observed in radio astronomy

a) Explain why the quantized angular momentum of a rotating molecule can be expressed as:

$$E(J) = \frac{J(J+1)\hbar}{2I}$$

Here *I* is the moment of inertia (*traagheidsmoment*) of a rotating di-atomic molecule. Use the property of the angular momentum operator J^2 to have eigen values: $J(J+1)\hbar^2$.

In radio astronomy spectral Lines are observed (in absorption or emission) of the CO (carbon monoxide) molecule making a transition from state J=1 to state J=0. This transition is at f=115.271208 GHz (Gigahertz, or 10^9 Hz). ($h=6.62606957 \times 10^{-34}$ Js).

- b) Calculate the separation R_e between the C-atom and the O-atom in the CO molecule. Use an expression for the reduced mass of the CO molecule (Masses $M_C = 12 \text{ a.m.u}$; $M_O = 15.994915$ a.m.u., with t 1 a.m.u. (atomic mass unit)= 1.660538921 x 10⁻²⁷ kilogram.)
- c) "Usual" ¹²C¹⁶O molecules consist of ¹²C and ¹⁶O atoms (isotopes). However, in radio astronomy also ¹²C¹⁸O molecules are observed. For the heavy oxygen molecule the mass is $M_O(18) =$ 17.999161 a.m.u. Make the assumption that the chemical bond in the ¹²C¹⁸O molecules is the same as for the main isotopomer ¹²C¹⁶O molecule. So assume that R_e has the same value for the heavier system.

Now calculate the frequency of the transition from J=1 to J=0 in the ¹²C¹⁸O molecule.