Physics of atoms and molecules

Assignment 2

Consider an atom with 1 valence electron.
Approximately consider the state of the valence electron ϕ_0 to have a constant value within a cube of sides 2 $\mathring{A}$ centered at the position of the nucleus (or ion in case there are core electrons) which is considered to be a point. This you can think of a scenario where an electron is detected by a single pixel of some detector with resolution 2 Å. Normalize ϕ_0.
Consider energy of the electron in such a state to be – 10 eV.
Consider a molecule formed by two such atoms at proximity 1.5 Å in the X direction.
Let β be -5 eV which is generally reasonable for 2s electrons.
Consider excitation of an electron from the ground state of the two atom system to the available excited state (as you saw in assignment 1 A). Note that there you got only one excited state because you consider a basis made of only two states (approximated to be orthonormal). In principle there are of course infinite number of excited states.

Calculate $| \, r_{21} \, |, \; \omega_{21}$ and estimate transition W_{21}^{D} rate we derived in the class and make an estimate of number of transitions which may be occurring in a second at room temperature.
Note that in deriving expression for $\rho(\omega)$ in class we have populated the entire phase space with photons. So we are essentially talking of the maximum possible values.

For the given system, how much time of exposure to the appropriate EM radiation is required for the population of the excited and ground states to be equal if there are only the stimulated processes (emission as well as absorption) in action at room temperature. Consider of course that the system was entirely in the ground state before exposure to the required EM field.