Mid-Semester Examination

Spectroscopy Monsoon-2023 (90 mins)

(1) Given time series of atomic velocities in a closed system containing N particles, write a pseudocode to compute the velocity autocorrelation function of the system. What can we infer from this time correlation function? How is it related to the vibrational density of states of the system? [3+1+1]

(2) (a) What is Frank-Condon principle?
(b) Discuss electronic absorption spectroscopy. [1+3]

(3) (a) Calculate the rotational energy levels allowed to the rigid diatomic molecule.
(b) What is the selection rule for a rigid diatomic molecule to show rotational spectrum?
(c) Diatomic molecules such as CO, HF will show a rotational spectrum whereas N_2, O_2, and H_2 do not. Why? If so, how do we determine the frequencies corresponding to rotational transitions. [5+1+2]

(4) Consider a ligand (L) binding to a protein (P) as shown in the figure. The natural vibrational frequencies of P and L are also provided in the figure. Using normal mode analysis, examine how the vibrational frequencies vary with the coupling between the protein and the ligand. [4]
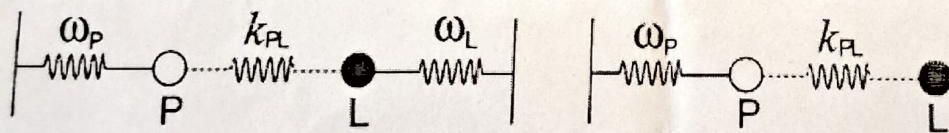
(5) Discuss the selection rules for vibrational transitions of a diatomic molecule using the harmonic oscillator model. [6]

(6) What is fluorescence spectroscopy? Discuss two of its applications in biophysics. [2+4]