Problem set 1: Computational Molecular Physics and Methods of Molecular Simulations

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(Please send the solution by e-mail to **tahereh.ghane@gmail.com** by **Fri. 24.04 (2pm)** at the latest.)

1 Balls in Boxes

(20 points) Determine the number of ways of placing three balls in three numbered boxes for each of the following cases:

(a) The balls are distinguishable with a limit of one ball per box.

(b) The balls are distinguishable with no limit on the number per box.

(c) The balls are indistinguishable with a limit of one ball per box.

(d) The balls are indistinguishable with no limit on the number per box.

Show the possible distributions for each case in the most clear way (table, graph, ...) on your choice.

2 Micro- and Macrostates

(20 points)
1- Consider 6 distinguishable particles and 2 energy levels (one with a degeneracy of 2 and the other with a degeneracy of 5).

(a) Calculate the number of macrostates and microstates in this system.

(b) Determine which macrostate is the most probable one.

2- Consider 6 distinguishable particles and 5 energy levels, each separated by ΔE. Particles are interacting weakly, i.e. they exchange energy but do not affect each other's energy levels. In the first 3 levels (i) a particle moves from 3rd level down to the 2nd level and (ii) a particle moves from 1st level to the 2nd level. In this case, the change in energy is balanced by exchange of particles for the 2 processes. Find all sets of occupation numbers of different energy levels.

3 Thermodynamic Quantities

(10 points) Use the partition function to derive the following thermodynamic function: (Entropy) $S = k_B ln\Omega$