

## 4.12: Ensemble Problems II

The remaining problems in this chapter deal with the same “principles” issues that the others do, but they assume some familiarity with physical and mathematical topics that we have not yet treated. I place them here because of their character, but I do not expect you to do them at this moment. Instead I list their prerequisites and I hope you will come back to them later.

### 4.18 The grand- $\omega$ ensemble for the simple harmonic oscillator

(Prerequisite: Problems 4.15 and 5.7.) Problem 4.15 introduced a class of ensembles in which mechanical parameters in the Hamiltonian were not fixed but rather allowed to fluctuate under the control of some parameters  $\gamma$ . Apply this concept to the diatomic molecules of problem 5.7, using the natural frequency of vibration as the mechanical parameter. Develop the suggestive arguments of problem 4.15 into a mathematically rigorous proof.

### 4.19 Particles in a bowl

(Prerequisite: Chapter 5.) I can’t count how many times I’ve waved my hands and told you that the precise character of the boundaries should be irrelevant to the bulk properties found by statistical mechanics. Now you have a chance to prove it (for a restricted situation of course).

- Consider  $N$  non-interacting, classical point particles moving subject to the potential energy function  $U(\mathbf{r}) = Kr^2/2$ . Evaluate the classical partition function  $Z_b(T, K, N)$  and compare it to the partition function  $Z_h(T, V, N)$  for  $N$  particles in a hard-walled container of volume  $V$ .
- For what  $V$  (as a function of  $K$ ) will the two partition functions in part (a.) be the same?
- The “bowl” container has no stiff walls, so it is possible for a particle to be located at any distance from the origin. But is it not likely that a particle will get too far away. Calculate the rms radius  $\sqrt{\langle r^2 \rangle}$ . (Use equipartition?)
- Suppose the hard-walled container is spherical with radius  $R$ . Place the origin at the center of the sphere and find the rms radius  $\sqrt{\langle r^2 \rangle}$ .
- For the  $V$  corresponding to  $K$  in the sense of part (b.), compare the two rms radii.

*Extra:* Do this problem quantum mechanically. (Clue: Notice the mathematical similarity between this problem and the Einstein model of lattice vibrations.)

### 4.20 Quantal monatomic ideal gas

(Prerequisite: Chapter 6.) We have many times considered the problem of  $N$  non-interacting classical point particles in a box of edge length  $L = V^{1/3}$ . Now we will solve the problem for quantum mechanical particles.

The partition function is  $Z = \sum e^{-\beta E}$ , where the sum is taken over the many-particle energy eigenstates  $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$ . Ignore symmetry-under-interchange requirements so that such states are specified by a simple listing of the component one-particle levels (or orbitals)  $\eta_k(\mathbf{r})$ . Thus  $\Psi$  can be specified by simply listing the relevant  $\mathbf{k}$  values of its component levels. Show then that

$$Z = \frac{1}{N!} \left( \sum_{\mathbf{k}} e^{-\beta E_{\mathbf{k}}} \right)^N \quad (4.12.1)$$

where  $E_{\mathbf{k}} = \hbar^2 k^2 / 2m$  and the sum is over all  $\mathbf{k}$  permitted by periodic boundary conditions. Evaluate the sum (in the thermodynamic limit) by turning it into an integral. Compare the resulting partition function with that of a classical monatomic ideal gas.

### 4.21 Quantal monatomic ideal gas in the microcanonical ensemble

Consider the situation of the above problem but calculate the microcanonical partition function  $\Omega(E, V, N)$ . Compare with the classical result.

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