Department of Physics
Preliminary Exam January 3–7, 2012
Day 4: Thermodynamics and Statistical Physics
Saturday, January 7, 2012
9:00 a.m. − 12:00 p.m.

Instructions:

1. Write the answer to each question on a separate sheet of paper. If more than one sheet is required, staple all the pages corresponding to a *single* question together in the correct order. But, do *not* staple all problems together. This exam has *six* questions. Select the *five* you want graded and *mark an "X"* through the problem you don't want graded.

2. Be sure to write your exam identification number (*not* your name or student ID number!) and the problem number on each problem sheet.

3. The time allowed for this exam is three hours. All questions carry the same amount of credit. Manage your time carefully.

4. If a question has more than one part, it may not always be necessary to successfully complete one part in order to do the other parts.

5. The exam will be evaluated, in part, by such things as the clarity and organization of your responses. It is a good idea to use short written explanatory statements between the lines of a derivation, for example. Be sure to substantiate any answer by calculations or arguments as appropriate. Be concise, explicit, and complete.

6. The use of electronic calculators is permissible and may be needed for some problems. However, obtaining preprogrammed information from programmable calculators or using any other reference material is strictly prohibited. Oklahoma State University Policies and Procedures on Academic Integrity will be followed.

*Do **only five (5)** (any five) of the six problems.*
***Mark an "X"** through the problem you don't want graded.*
Each graded problem carries 20 points.

Boltzmann's constant: $k_B = 1.38 \times 10^{-23}$ J/K

Gas constant: $R = 8.31$ J/(mol·K)

Unified mass unit: $u = 1.66 \times 10^{-27}$ kg

Gaussian integrals:

$$\int_0^\infty \exp(-\lambda x^2)\,dx = \frac{1}{2}\sqrt{\frac{\pi}{\lambda}} \qquad \int_0^\infty x^3 \exp(-\lambda x^2)\,dx = \frac{1}{2\lambda^2}$$

$$\int_0^\infty x \exp(-\lambda x^2)\,dx = \frac{1}{2\lambda} \qquad \int_0^\infty x^4 \exp(-\lambda x^2)\,dx = \frac{3}{8}\sqrt{\frac{\pi}{\lambda^5}}$$

$$\int_0^\infty x^2 \exp(-\lambda x^2)\,dx = \frac{1}{4}\sqrt{\frac{\pi}{\lambda^3}} \qquad \int_0^\infty x^5 \exp(-\lambda x^2)\,dx = \frac{1}{\lambda^3}$$

Problem 1

(a) From *macroscopic* thermodynamics, show that:

$$U = F - T\left(\frac{\partial F}{\partial T}\right)_V = -T^2\left(\frac{\partial (F/T)}{\partial T}\right)_V$$

(b) From *statistical* thermodynamics, show that:

$$\langle E \rangle \equiv \frac{\sum_i E_i e^{-E_i/k_B T}}{\sum_i e^{-E_i/k_B T}} = \frac{1}{Q}\frac{\partial Q}{\partial(\frac{-1}{k_B T})}\bigg|_V = k_B T^2\left(\frac{\partial(\ln Q)}{\partial T}\right)_V$$

(c) Comparing the above results, deduce the relation between the Helmholtz free energy (F) and the canonical partition function (Q).

Problem 2

Entropy for system of identical noninteracting fermions.

(a) *Derive*, from an appropriate partition function, the following general expression for the entropy of a system in thermodynamic equilibrium made up of identical, noninteracting fermions (e.g., a free-electron ideal gas):

$$S = -\sum_i k_B \left[f_i \ln f_i + (1 - f_i) \ln(1 - f_i) \right],$$

where

$$f_i \equiv \frac{1}{e^{(\varepsilon_i - \mu)/k_B T} + 1} \qquad \text{(Fermi–Dirac distribution)}$$

and the sum is over all *single-particle states* (labeled by i). All symbols have their usual meanings.

(HINT: Grand canonical partition function, written for a particular single-particle state i of energy ε_i.)

(b) Let $S_i \equiv -k_B \left[f_i \ln f_i + (1 - f_i) \ln(1 - f_i) \right]$ denote the entropy of just the ith single-particle state by itself. (Obviously, $S = \sum_i S_i$.) Evaluate S_i for the following cases:
  - $f_i = 0$
  - $f_i = 1$
  - Can S_i ever be < 0? What is the value of $S_i^{\max}$?

(c) Interpret the meaning of the results in part (b).

(d) Without doing additional calculation: What would the total entropy, S, be for the case where the occupancy (0 or 1) of *each* single-particle quantum state is known with *certainty*? Can you give a physical example which well approximates such a situation? What happens to S when one or more occupancies become *uncertain*?

Problem 3
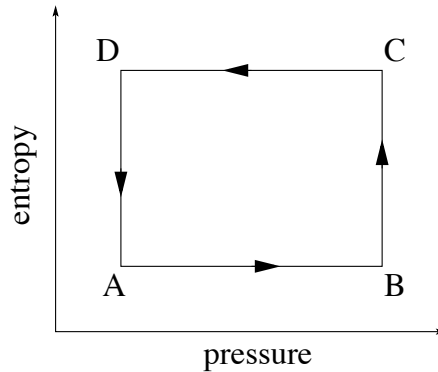
Heat engine. The Brayton cycle is shown in the S-P diagram. Assume that the working substance is an ideal gas.

(a) Show which is/are the heat absorbing process(es), and determine the amount of heat absorbed;

(b) Show which is/are the heat expelling process(es), and determine the amount of heat expelled;

(c) Calculate the efficiency of the cycle expressed in pressures P_A and P_B and heat capacities C_P and C_V.

(d) Draw the P-V diagram of the cycle (V as x-axis). Label the corners with letters A–D consistent with the ones given in the S-P diagram.

(e) Draw the T-S diagram of the cycle (S as x-axis).

Problem 4

Application of Maxwellian distribution. The speed of O_2 molecules in a container follows the Maxwell distribution $f(v) \propto v^2 e^{-mv^2/2kT}$. The number of molecules with speed v that hit the wall in a given time is proportional to the speed v and to $f(v)$. Assuming there is a very small hole in the wall (too small to affect the distribution inside), the speed distribution of those molecules that escape is $F(v) \propto v f(v)$.

(a) Calculate the average speed for O_2 molecules inside the box, assuming $T = 300\,\mathrm{K}$.

(b) Calculate the average speed for the O_2 molecules that escape. How does this compare to the average speed of molecules inside the box? Justify your result.

(c) Calculate the mean translational kinetic energy of those that escape. How does this energy compare to the mean translational kinetic energy for molecules inside the box as predicted by the equipartition theorem? Also justify your result.

Problem 5
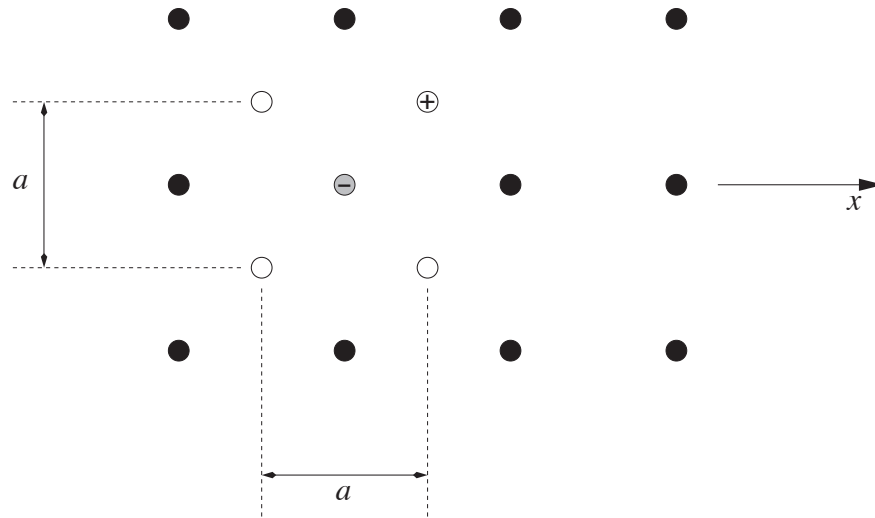
Model of polarizability on a lattice. The following describes a simple two-dimensional model of a situation of actual physical interest.

A solid at temperature T contains N negatively charged impurity ions per cm^3, these ions replacing some of the ordinary atoms of the solid. The solid as a whole is, of course, electrically neutral. This is so because each negative ion with charge $-e$ has in its vicinity one positive ion with charge $+e$. The positive ion is small and thus free to move between the lattice sites.

In the absence of an external electric field it will, therefore, be found with equal probability in any one of the four equidistant sites surrounding the stationary negative ion (see diagram; the lattice spacing is a).

If a small electric field E is applied along the x direction, calculate:

(a) The probability that the positive ion will be in one of the right-side positions.

(b) The electric polarization, i.e., the mean electric dipole moment per unit volume along the x direction.

(c) What is the expected value of the electric polarization when the temperature is very low or very high?

Additional information:

- Electric dipole moment is $\mathbf{p}=q\mathbf{r}$, where $\mathbf{r}$ is the vector position from the negative to the positive charge and q is the charge of the electron.

- Energy of an electric dipole in an electric field is $\varepsilon=-\mathbf{p}\cdot\mathbf{E}$.

Problem 6

Lattice vibrations in the Einstein model. A crystalline solid can be modeled as an assembly of $3N$ identical, independent harmonic oscillators. The molecular partition function for each oscillator is given by:

$$\zeta = (1 - e^{-\theta_{\mathrm{E}}/T})^{-1}$$

where θ_{E} is a relevant Einstein temperature.

(a) Determine the canonical partition function for this solid.

(b) Derive suitable relations for its internal energy and entropy.

(c) What is the chemical potential for this crystalline solid?