

**FINAL EXAM**

- You have 180 minutes
- You are permitted to have one letter-sized sheet of hand-written notes
- No other references or electronic devices are permitted

Each problem on this exam has multiple parts (a, b, c, ...). Some parts can be done out of sequence. If you get stuck on one part, still look at the rest of the problem!

1. *Diatomic molecules* (15 points). In a certain range of temperatures, a diatomic molecule is well approximated as a rigid rotor with moment of inertia  $I$ . Its energy eigenstates are

$$\varepsilon_{\ell,m} = \frac{\ell(\ell+1)\hbar^2}{2I} \quad (1)$$

with  $\ell = 0, 1, 2, \dots$ . For each value of  $\ell$  there are  $2\ell + 1$  degenerate states labeled by integers  $m$  (with  $|m| \leq \ell$ ).

- a. State a condition on the temperature  $\tau$  for the molecule to be in a classical regime.
- b. Calculate the following properties of the molecule as a function of temperature  $\tau$  in the classical regime:
  - i. ... the Helmholtz free energy
  - ii. ... the entropy
  - iii. ... the average energy
- c. Based on physical arguments, what is the limiting value of the entropy as  $\tau \rightarrow 0$ ?

2. *Hydrogen in equilibrium* (25 points). A hydrogen molecule can dissociate into two hydrogen atoms via the reaction



Consider a chamber of volume  $V$  containing  $N_A$  hydrogen atoms and  $N_M$  molecules of  $\text{H}_2$  at temperature  $\tau$ .

- State a condition on the chemical potentials  $\mu_A$  of the atomic gas and  $\mu_M$  of the molecular gas for the reaction to be in equilibrium.
- You previously derived the chemical potential

$$\mu_A = \tau \ln \left( \frac{N_A \lambda_{\tau,A}^3}{V} \right) \quad (3)$$

for a monatomic gas, where  $\lambda_{\tau,A}$  is the thermal de Broglie wavelength. How is the thermal de Broglie wavelength  $\lambda_{\tau,M}$  of the molecules related to that of the atoms at equal temperature  $\tau$ ?

- Find the chemical potential of the gas of hydrogen molecules. Regard each molecule internally as a classical rigid rotor (Problem 1.b.) with moment of inertia  $I$  and binding energy  $E_b$ . (The binding energy is the energy difference between two isolated hydrogen atoms and a hydrogen molecule in its internal ground state.)
- Find the equilibrium ratio  $N_M/N_A^2$ . Express your result in terms of  $\tau$ ,  $\lambda_{\tau,A}$ ,  $V$ ,  $E_b$ , and  $I$ .
- Answer each of the following questions with a *physical interpretation*:
  - As the volume  $V$  is increased, does the equilibrium ratio  $N_M/N_A^2$  increase, decrease, or remain the same?
  - For a molecule  $X_2$  with a higher binding energy than  $\text{H}_2$ , all else being equal, would the equilibrium ratio  $N_M/N_A^2$  be higher, lower, or the same?
  - For a molecule  $X_2$  with a higher moment of inertia than  $\text{H}_2$ , all else being equal, would the equilibrium ratio  $N_M/N_A^2$  be higher, lower, or the same?

3. *Bose-Fermi Mixture* (40 points). A mixture of  $N_f$  identical fermions and  $N_b$  identical bosons is trapped in a three-dimensional harmonic potential. The trapping potential is the same for both species, with single-particle energy eigenstates:

$$\varepsilon(n_x, n_y, n_z) = (n_x + n_y + n_z)\hbar\omega. \quad (4)$$

The bosons and fermions are in equilibrium at temperature  $\tau$ . Throughout this problem, we will examine how the properties of the system **scale** with parameters such as  $N_b, N_f, \hbar\omega$ , and  $\tau$ . You need not calculate numerical prefactors, but you must clearly show how you arrive at each answer.

- a. Sketch a surface of constant energy  $\varepsilon$  as a function of  $n_x, n_y, n_z$ .
- b. How does the density of states  $\mathcal{D}(\varepsilon)$  in the harmonic trap scale with energy  $\varepsilon$  and trap frequency  $\hbar\omega$ ?
- c. *Fermi degeneracy*:
  - i. Find the scaling of the Fermi energy  $\varepsilon_F$  with  $N_f$  and  $\hbar\omega$ .
  - ii. Give a condition on the temperature  $\tau$  for the Fermi gas to be in the quantum degenerate regime.
- d. *Bose-Einstein condensation*:
  - i. Show that Bose-Einstein condensation can occur in the 3D harmonic trap.
  - ii. How does the critical temperature  $\tau_E$  for Bose-Einstein condensation scale with  $N_b$  and  $\hbar\omega$ ?
- e. From now on, assume that the temperature is in the regime  $\hbar\omega \ll \tau \ll \tau_E, \varepsilon_F$ . Find the scaling of the following quantities with  $N_{b/f}, \hbar\omega$ , and/or  $\tau$ :
  - i. The total energy  $E_b$  of the Bose gas
  - ii. The heat capacity  $C_b$  of the Bose gas
  - iii. The total energy  $E_f$  of the Fermi gas
  - iv. The heat capacity  $C_f$  of the Fermi gas
- f. *Evaporation*. After preparing an ultracold mixture of Bose and Fermi gases, you wish to cool it further. To this end, you remove all bosons with energy  $\varepsilon > \eta\tau$ . Sketch the number of bosons per unit energy vs.  $\varepsilon$ , shading in a region of area  $\Delta N_b \ll N_b$  representing the number of bosons removed. Give a condition on  $\eta$  to ensure that the fraction of bosons removed is small.
- g. *Sympathetic cooling*. After removing the most energetic bosons, and therewith an energy  $\epsilon_1 \Delta N_b$ , you let the Bose and Fermi gases equilibrate to a new temperature  $\tau - \Delta\tau$ . Find the temperature change  $\Delta\tau/\varepsilon_F$  in units of the Fermi energy, as follows:
  - i. The net effect of the cooling process is to reduce the energies of the Fermi and Bose gases by  $\Delta E_f$  and  $\Delta E_b$ , respectively. How does the ratio  $\Delta E_f/\Delta E_b$  scale with  $N_{b/f}, \varepsilon_F$ , and/or  $\tau$ ? (Assume  $\Delta\tau \ll \tau$ .)
  - ii. Based on part i., in the quantum degenerate regime, does the cooling process extract more energy from the Bose gas or from the Fermi gas?
  - iii. How does the temperature change  $\Delta\tau/\varepsilon_F$  scale with  $N_{f/b}, \Delta N_b, \tau$  and/or  $\epsilon_1$ ?
- h. **Extra credit**: Suppose that you conduct the cooling process in f.-g. continuously, always removing any bosons with energy  $\varepsilon > \eta\tau$  as the system thermalizes. If you are willing to sacrifice a fixed fraction of the bosons, how should you choose the cutoff  $\eta$  and the initial ratio  $N_b/N_f$  of bosons to fermions to maximize  $\Delta\tau/\varepsilon_F$ ?

4. *The Otto Cycle* (30 points). Most automobile engines generate work through the Otto cycle, which consists of the following four processes:

- (1) Adiabatic compression
- (2) Isometric heating (that is, heating at constant volume)
- (3) Adiabatic expansion
- (4) Isometric cooling (cooling at constant volume)

- a. Show that for an ideal gas,

$$\tau = \alpha(N, V) \cdot e^{\frac{2}{3} \frac{\sigma}{N}}$$

where  $\alpha$  is independent of temperature.

- b. Draw a  $\tau - \sigma$  diagram for the Otto cycle with the following assumptions:

- i. The working fluid is an ideal gas with no internal degrees of freedom.
- ii. Before adiabatic compression, the temperature is  $\tau_0$ .
- iii. The temperature rises from  $\tau_0$  to  $2\tau_0$  during adiabatic compression.
- iv. The temperature is  $4\tau_0$  after isometric heating.

Label each curve in the diagram with the corresponding process (1), (2), (3), or (4). Where any two curves intersect, label the  $\tau$  axis in terms of  $\tau_0$ , and label the  $\sigma$  axis in terms of  $\sigma_1$  (the entropy during adiabatic compression) or  $\sigma_3$  (the entropy during adiabatic expansion).

- c. Show that the work done in one Otto cycle is

$$W = \frac{3}{2} P_0 V_0.$$

Hint: use the  $\tau - \sigma$  diagram and the ideal gas law.

- d. One Otto cycle can be accomplished in  $\sim 1$  millisecond. Estimate the power output of an automobile engine of volume  $2 \cdot 10^{-3}$  cubic meters operating at atmospheric pressure ( $10^5$  Pa).
- e. Draw a  $P - V$  diagram for the Otto cycle with the same assumptions as in part b. Label each curve in the diagram with the corresponding process (1), (2), (3), or (4). Where any two curves intersect, label the  $P$  and  $V$  axes in terms of  $P_0$  and  $V_0$ , the pressure and volume before adiabatic compression.

5. *Microcanonical Entropy* (30 points). Boltzmann's definition of entropy, which we have used in this course, leads to incorrect predictions when applied to certain isolated systems. This problem will explore one such system.

Consider a single particle of mass  $m$  with energy  $E$  moving in a one-dimensional box of length  $L$ . The particle exerts a time-averaged force  $f$  on each wall of the box. We define  $f$  so that  $f$  is positive if the force on the wall is directed outward.

- Why must we have  $f > 0$ ? Find  $f(E, L)$  by treating the particle classically and calculating the momentum exchanged with one wall during one round trip.
- Now we will use quantum mechanics and thermodynamics to calculate  $f$ . What is the fundamental thermodynamic relation for this system?
- Show that

$$f = \tau \left( \frac{\partial \sigma}{\partial L} \right)_E.$$

- The  $n^{\text{th}}$  state of a particle in a 1D box has energy

$$\epsilon(n) = \frac{\hbar^2 \pi^2}{2mL^2} n^2.$$

Assume that there is some uncertainty  $\delta E$  in the energy of the particle, so that the energy is known to be between  $E - \delta E$  and  $E + \delta E$ . Furthermore, assume that  $\delta E$  is small compared to  $E$  but large compared to the energy spacing between adjacent states.

Calculate the multiplicity

$$g = \int_{E-\delta E}^{E+\delta E} D(\epsilon) d\epsilon,$$

where  $D(\epsilon)$  is the density of states. Approximate your result to first order in the small parameter  $\frac{\delta E}{E}$ .

- Calculate the entropy  $\sigma(E, L)$ . Invert this expression to find  $E(\sigma, L)$ .
- Calculate the temperature  $\tau(E)$ . What is unusual about your result?
- Calculate  $f(E, L)$  using the expression from part c. What is wrong with your result?
- Extra credit:** The *Gibbs entropy* is defined by

$$\sigma_G = \ln \int_0^E D(\epsilon) d\epsilon.$$

Repeat parts e, f, and g using this definition of entropy.